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RECENT PHYSICAL MODELLING DEVELOPMENTS IN A LAGRANGIAN MODELLING SYSTEM FOR EMERGENCY RESPONSE PURPOSES

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Abstract: Industrial accidents as malevolent or terrorist actions could result in undesirable atmospheric releases of noxious species, especially radionuclides or toxic chemicals. Relating to this societal and governmental concern, there is an increasing demand for modelling and decision-support systems dedicated to the emergency preparedness and response. The challenge is to provide the most precise and reliable evaluation of the space and time distribution of the deleterious gases or airborne particles, and moreover of their consequences on the environment and human health, in computation times consistent with a crisis management. First attempt responses supplied by Gaussian modelling are definitely limited in case of complex meteorological conditions and/or events likely to occur in the urban or industrial built environment. On the other hand, CFD still exhibits disqualifying computation scores. Micro-SWIFT-SPRAY developed by ARIA Technologies, ARIANET, MOKILI, and CEA is an intermediate quick response capability to simulate the micro-scale processes. Original physical models have been recently implemented in MSS, like a 3D pressure diagnosis used to evaluate the indoor/outdoor transfers and the generalization of dry deposition on all accessible surfaces (buildings facades, roofs or ceilings). These developments are depicted in the paper as is the briefly commented on, soon arriving parallel architecture of MSS which will enable dramatic reduction of the computation times and make MSS a really operational modelling system.

Key words: modelling and decision-support system, micro-scale, urban environment, 3D mass-consistent flow field, 3D Lagrangian dispersion model, pressure diagnosis, indoor/outdoor transfer, generalized deposition, parallel version, Micro-SWIFT-SPRAY.

INTRODUCTION

On one hand, national and European regulatory requirements regarding environmental and health impact assessment studies have become more and more stringent. It is also highly recommended to use reliable, fast running and as precise as possible simulation tools in the framework of emergency preparedness and response to accidental, or even malevolent atmospheric dispersal events.

On the other hand, in the recent years, there have been great developments in the domains of (1) meteorological flows and dispersion processes modelling, and (2) computing performances and speed (due to a more efficient programming with the development of parallel versions of codes, and the use of an increasing number of processors).

For regulatory purpose or in a first attempt in a crisis situation, the pollutants dispersion is usually computed using Gaussian plume or puffs 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 micro-scale, a CFD model adapted to the atmospheric boundary layer is the reference way of investigation, but it is extremely demanding in computational resources, especially for two important applications: long term impact around a source near the ground and emergency response or preparedness.

MICRO-SWIFT-SPRAY PRESENTATION

The previous considerations are incitements to compute the flow field without solving the Navier-Stokes equations and to evaluate the dispersion with a Lagrangian particles model. All of this can be found in Micro-SWIFT-SPRAY (MSS) modelling system which is developed by ARIA Technologies, ARIANET, and MOKILI, in partnership with the French Atomic Energy Commission. MSS is an intermediate quick response capability designed to simulate urban or industrial micro-scale flow and dispersion processes with CPU times significantly shorter than a full CFD solution.

MSS is the combination of Micro-SWIFT and Micro-SPRAY. Micro-SWIFT is a mass consistent diagnostic 3D wind model in which the aerodynamic effects due to the buildings are represented by analytical flow zones. The current Micro-SWIFT version, dubbed "NSWIFT", is able to deal with 3D nested computation domains having increasing horizontal resolutions. Micro-SPRAY is a 3D Lagrangian dispersion model taking account of the particles rebounds on buildings as well as local turbulence.

MSS has been validated in numerous and various configurations. In all cases, numerical results issued by MSS scored correctly or highly when compared with analytical solutions or experimental measurements. The validation cases include many dispersion tests conducted at a reduced scale in wind tunnels (for example, at Hamburg University) and real scale "in-field" experimental campaigns Urban 2 000 and Urban 2 003 which took place in Salt-Lake City, UT (USA) and Oklahoma City, OK (USA) (Sontowski *et al.*, 2004, and Harris *et al.*, 2007).

The MSS *modelling* system is now extensively used for accidental or deliberate releases of noxious species in the urban environment. In these applications, it is essential to evaluate together the concentrations, the depositions, and the radiological or chemical doses, in the streets network, and also inside the buildings. Relating to these topics, many development activities are in progress. The paper gives an overview of modelling improvements recently done in MSS. For each development, we provide some technical details including validation cases based on comparisons with experiments or numerical results issued by other models, and discuss practical applications illustrating MSS response capabilities to realistically simulate 3D flow field and indoor/outdoor dispersion processes.

NSWIFT 3D PRESSURE FIELD DIAGNOSTIC

To estimate species concentrations both, outdoor, in the built environment of a city or an industrial site, and indoor, in the buildings, it is necessary to compute the 3D pressure field due to the wind field. NSWIFT has been supplemented with a pressure solver. Using mass balance and Navier-Stokes equations of an uncompressible flow, assuming that each variable is the sum of an ensemble average (denoted by a line) and a fluctuation, and neglecting the Reynolds stresses, the 3D pressure field verifies equation (1) where ρ designates the density, p the pressure and U the velocity.

$$\Delta\bar{p} = -\rho \,\mathrm{div}\, \partial_j(\bar{U}_j\bar{U}_i) \qquad (1)$$

$$C_p = \frac{\bar{p} - \bar{p}_0}{0.5\,\rho\,U^2} \qquad (2)$$

The 3D pressure field is diagnosed by solving the Poisson equation (1) which is similar to the equation used to satisfy the mass consistency of the interpolated 3D wind field in NSWIFT. The only difference relates to the boundary conditions. For the pressure equation, Neumann relation $\nabla p.\underline{n} = 0$ is used with $\underline{n}$ the unit boundary normal vector.

For validation purpose, the numerical results issued by NSWIFT pressure solver were compared with wind tunnel experimental results and/or with the pressure fields computed by QUIC, a 3D wind field diagnostic model, similar to NSWIFT, developed in the United States, at Los Alamos National Laboratories (LANL). Many validation cases have been carried out with various geometries: a cube with upstream side normal or 45° incident wind, tall, low flat or L-shaped buildings, and a 2D-array of seven wide buildings. It was noticed that the pressure on the buildings walls strongly depended on wind field preciseness near the obstacles, so the influence of the upwind displacement zones and canyon zones was studied, and a rooftop recirculation was implemented in NSWIFT.

The pressure coefficient (2) along the sides of a cube was compared with the "small" scale test performed in 2001 at Silsø Research Institute. In this experiment, the atmosphere was neutral and the wind blew normally to a 6 m edge cube upstream side (speed of 9.5 $m.s^{-1}$ at 6 m height). NSWIFT was also compared with Baines date (Baines, 1963) obtained in Toronto University wind tunnel and, finally, with QUIC pressure solution (Gowardhan *et al.*, 2005). Figure 1 presents these results and NSWIFT pressure diagnosis which is the best using Brown (*vs.* Röckle) upwind displacement zone and taking account of the rooftop recirculation.

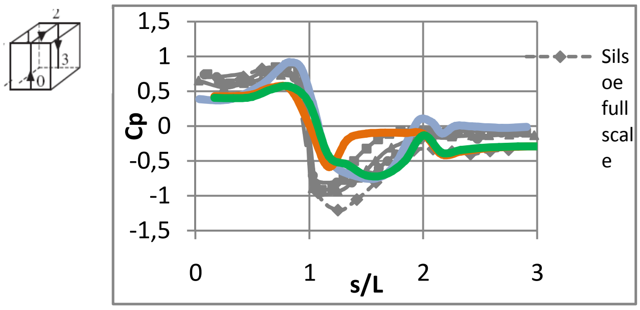

Figure 1. Pressure coefficient along the sides of a cube. Comparison of experimental and QUIC results with NSWIFT pressure solution.

US-EPA data (Brown *et al.* 2001) were used in order to evaluate NSWIFT pressure diagnosis in a canyon geometry exhibiting seven parallel buildings (length: width: height = 3.7: 0.15: 0.15, space between each block = 0.15). In the experiment, the atmosphere was neutral and the wind perpendicular to the obstacles. A new parametrization of the skimming zone, called CPB-PAR (Hotchkiss and Harlow, 1973), was introduced in NSWIFT. As it can be seen in Figure 2 comparing numerical and experimental results, NSWIFT satisfies to reproduce the detail of the wind field around the first obstacle, especially the vortex inside the canyon zone. The pressure field is correctly diagnosed by NSWIFT on the front side, but slightly under-estimated at the rear of the obstacle.

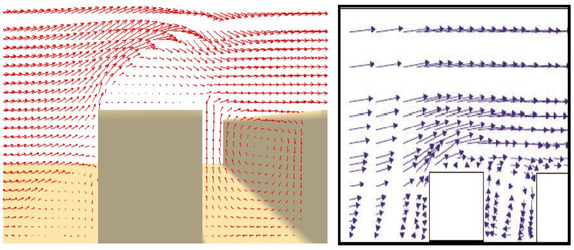

Figure 2. Wind field issued by NSWIFT (left) and measured in a wind tunnel (right) in the vicinity of the first parallelepipedic obstacle in a 2D array of seven.

The numerous validation cases demonstrate that NSWIFT pressure solver gives excellent results on buildings upwind sides and satisfying results on the flat roofs where the rooftop recirculation noticeably improves the pressure diagnosis. In these regions, the pressure gradients are mainly governed by the mean wind. On the lateral and back sides, NSWIFT calculations are less consistent with the measurements. This can be explained by the insufficient recirculation along the lateral sides and the not fully satisfying wake zone model disregarding the Reynolds stresses. Comparing NSWIFT and QUIC pressure solution, NSWIFT gives results at least as good as QUIC, or better in some cases.

POLLUTANTS TRANFER INSIDE AND OUTSIDE THE BUILDINGS

Contamination infiltration inside the buildings is a crucial process to deal with in order to estimate the health effects on public or rescue teams of both chronic, and even more, accidental or malevolent releases. Concentrations entering a building depend on its ventilation and airtightness, and on the species properties and distribution near the building façades. Linked to the surface pressure distribution on buildings frontages, the interior concentrations can now be computed by MSS in which an inflow/outflow scheme was implemented. The concentrations are assumed uniform in the volume of each obstacle and estimated according to three methods.

Method #1 – The buildings are considered as "low-pass filters" (by analogy with electrical R-C circuits). The interior concentration is a function of the atmospheric mean concentration and of an infiltration constant which is an overall air renewal duration (associated with each building). The infiltration parameter is set for different buildings blocks as texture attributes in a GIS (shape file). There is no entrance of particles, nor exit of the contaminant. Infiltration has no influence on any external concentration depletion. Despite being very simple, this approach gives a good comparison between MSS and the analogous infiltration model in the emergency response code ALOHA, developed by US-EPA.

Method #2 and #3 – All the virtual particles dispersed in the atmosphere have a probability to enter the obstacles where they stay till being expelled. The infiltration probability is the probability for each particle to be physically in the inflow air which is determined from the infiltration time constant, the obstacle volume, and the fluid meshes volumes. The 3D pressure field diagnosed in NSWIFT controls the mass inflow and outflow. The particles infiltrate (resp. leave) through the sides with positive (resp. negative) pressure difference. In method #2, the air is supposed to enter the buildings only through the meshes with positive pressure difference. This is the most precise approach. In method #3, the air is assumed to penetrate the buildings through all sides without consideration for the sign of the pressure difference. This approach is less rigorous but it gives results comparable to the method #1 and it validates the use of the pressure diagnosis and of the probabilistic approach.

Figure 3 illustrates the infiltration in buildings blocks (with different infiltration parameters) of the traffic emissions in Paris real urban landscape. This work was a first attempt to introduce the indoor/outdoor transfers in MSS. It has some identified limitations. For example, the infiltration "constant" should also depend on the wind field around the obstacle, the temperature gradient between inside and outside, and the obstacle characteristics. One way to cope with this problem could be to use not only qualitatively, but also quantitatively, NSWIFT pressure diagnosis. More precise data about the buildings should also be taken into account to evaluate their airtightness.

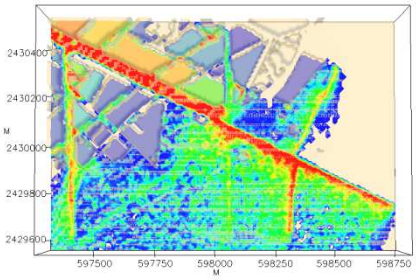

Figure 3. Concentrations due to the traffic emissions in the streets network and inside the buildings in a district of Paris (France).

MICRO-SPRAY GENERALIZED DEPOSITION PROCESSES

To take account of the deposition on all surfaces while dispersing gaseous or particulate airborne contaminants is a major issue. As a matter of fact, the dry or wet depositions result in depleting the plume and creating contamination spots on all accessible surfaces. In the case of radionuclides releases, it is especially important to know these spots to precisely evaluate the radiological exposure by irradiation. In Micro-SPRAY, the depositions have been generalized as these processes can now be computed not only on the ground, but also on complex surfaces like buildings facades, roofs, and ceilings of covered structures: tunnels, walkways, arches...

Dry deposition

In Micro-SPRAY, dry deposition on the ground is evaluated using a probabilistic approach, derived from Boughton and Delaurentis (1987). The Lagrangian particles corresponding to gaseous species are depleted gradually as they settle. For the aerosols, a random number is drawn; if it is less than the ground deposition probability computed by Micro-SPRAY, the "whole" particle settles; if not, it does not settle. Boughton and Delaurentis model was extended and complementary deposition probabilities were defined on the walls, roofs, and on the eastern, western, northern and southern frontages.

The particles deposition probabilities are functions of the distance to the obstacle, the local turbulence and the species deposition velocity. If a particle is surrounded by obstacles together east, west, north, and south, it can settle on the four surfaces, also on a ceiling or roof, or on the ground. As it would bias the results of the stochastic model to force the deposition sequence, three random drawing methods have been tested in Micro-SPRAY to determine the order of deposition on the different surfaces. With a sufficient number of particles, all methods converge to a unique solution.

The method adapted both to gases and aerosols was adopted. At each time step, a particle can settle only on one surface. The deposition probabilities in the seven directions are distributed proportionally along an interval between 0 and 1. A random number is drawn in the same interval and determines on which surface the deposition takes place. The more the deposition probability in a direction is high, the more deposition on this surface is obtained.

Dry deposition computations have been performed first using simple academic geometries, then in the more complex situations of urban districts. Figure 4 shows separately the depositions on the frontages and roof of a 50 m edge cubic obstacle. The wind blows normally to the cube (5 $m.s^{-1}$ speed at 10 m height). The source is punctual, located upstream of the obstacle. In the example, the deposition velocity is set to zero on the ground. On the façades and roof, it is equal to 0.1 $m.s^{-1}$. As each particle is able to settle only on one surface, it is verified that the depositions drawing methods give identical results. Figure 5 presents an extended realistic configuration including numerous buildings. Sources are linear, at 1 m above the streets level, and correspond to the traffic emissions. With enough particles, depositions on the surfaces do not depend on the drawing methods. Finally, emissions inside tunnels were studied. In this case, the particles are likely to settle on the walls, ceiling and ground. Calculations were carried out in a 100 m long tunnel with a point source in the middle and the wind in the axis of the tunnel.

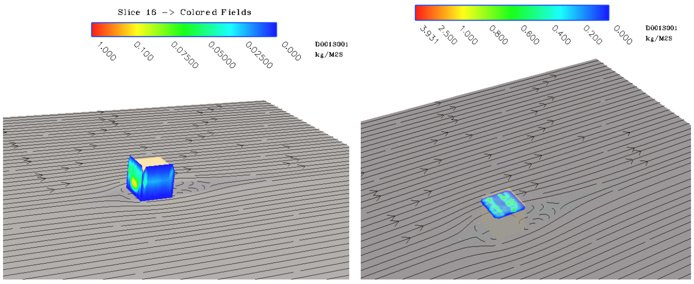

Figure 4. Dry depositions on cube sides. Streamlines are shown as depositions on the façades (left) and roof (right).

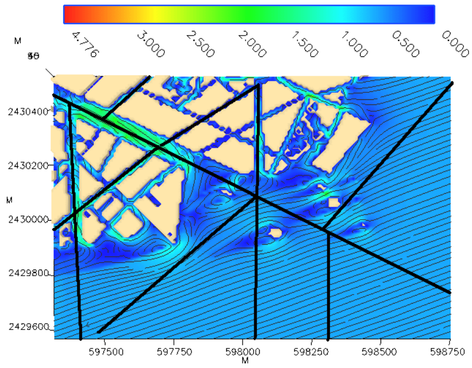

Figure 5. Location of real urban district buildings. Streamlines and velocity field at 2 m above the ground level. Black lines figurate traffic emissions.

For the storage of the dry depositions, both 2D and 3D fields are used to distinguish between the results on the ground and on the obstacles walls, roofs and ceilings. Dry deposition velocities on the surfaces are defined three different ways: they can be the same in the whole domain for a given species, or specified by areas, or related to buildings texture attributes defined in a GIS (shape file) of which Figure 6 is an example. It is considered to constitute a data base of deposition velocities of various species on typical urban surfaces (concrete, stone, brick, wood), but to our knowledge, there are few available data in published works.

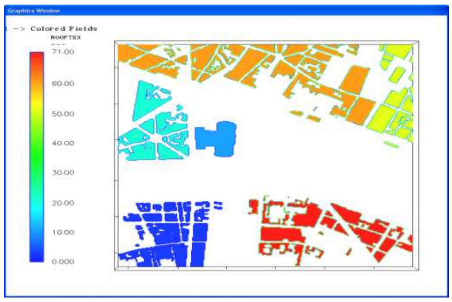

Figure 6. Horizontal section of the roofs textures in a district of Paris (France)

Wet deposition

Wet deposition was also up-graded to take account of obstacles and structures like arches or bridges. Figure 7 shows an example of generalized geometry which MSS is now capable of coping with. Wet deposition is a physical process resulting in plume depletion due to the rain. In Micro-SPRAY, it is represented using a washout coefficient depending on the species and precipitation intensity. The particles protected against washout by a ceiling are not deposited. The shielding effect has been tested in the above introduced tunnel configuration. Particles are released in a tunnel where they disperse (with no exit out of the tunnel). In the same time, it is raining outside. In this case, there is no deposition. On the contrary, if the tunnel vault is removed, there is wet deposition as can be seen and compared in Figure 8. Finally, let’s mention that wet deposition on buildings facades is not yet available in Micro-SPRAY. It certainly depends on the rain drops incidence and could be a future development.

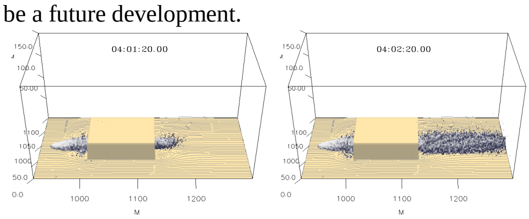

Figure 7: Example of a hollow geometry in MSS

Figure 8: Evaluation of wet deposition in a tunnel geometry with (left) or without (right) a vault.

CONCLUSION AND PERSPECTIVES

Micro-SWIFT-SPRAY *modelling* system is used to evaluate the 3D flow field and gases or aerosols dispersion at the micro-meteorological scale, in complex urban or industrial environments. MSS applies essentially for short duration releases, but also for long term impact emissions. This paper focuses on original functionalities recently implemented in MSS, especially useful in case of accidental or malevolent events implying deleterious releases in a built area. The contamination space and time distribution is available not only in the streets network, but potentially toxic interior concentrations inflow/outflow can be computed using the pressure field diagnosed around the obstacles by NSWIFT. Moreover, Micro-SPRAY was generalized to determine the dry depositions on all accessible external surfaces, *i.e.* the ground as the buildings façades and roofs. MSS is now able to take account of hollow geometries like bridges, arches, walkways and tunnels, and also, the shielding effect against the washout by the rain, if any.

MSS was conceived as the compromise of a simplified CFD solution and a quick response *modelling* system. It was formerly tagged as "90% of the solution for less than 10% of the CPU". Various validation and application exercises have shown that it is the case. Indeed, comparisons with Navier-Stokes solving CFD codes have demonstrated that MSS gives very good results in reduced computation times. The next step in MSS development is now to elaborate a parallel architecture of the system. It is called PMSS and combines parallel time frames and tiles (sub-domains) in Micro-SWIFT and parallel particles clouds for each tile in Micro-SPRAY. This in progress action is performed by ARIA Technologies, MOKILI and CEA. The target configurations are principally Windows and Linux computers clusters, operating moderate to huge numbers of processors (quadricore or octocore to more than 3 500 processors at CEA DAM Île-de-France). It is foreseen to dramatically decrease the computation times.

Computing the space and time atmospheric dispersion with adequate consideration for buildings effects and indoor/ outdoor transfers, assessing the surface contamination and, later, the health impact, all of this in real or accelerated time, should make PMSS a *modelling* system adapted to the decision-support and emergency response.

REFERENCES

Baines, W., 1963: Effects of velocity distribution on wind loads and flow patterns on buildings. The symposium on wind effects on buildings and structure. Middlesex, England (UK). National Physical Lab.1, 197-225.

Boughton, B.A., J.M. Delaurentis, W.E. Dunn, 1987: A stochastic model of particle dispersion in the atmosphere. Boundary Layer Meteorology, vol. 40, pp 147-163.

Brown, M.J, *et al.*, 2001: Many-building wind tunnel experiments. Los Alamos National Laboratory.

Gowardhan, A.A., M.J. Brown, D.S. Decroix, and E.R. Pardyjak, 2005: Evaluation of QUIC pressure solver: comparison to wind-tunnel measurement. Los Alamos National Laboratory, Los Alamos, NM. University of Utah, Salt Lake City, UT (USA).

Harris, T., C. Dougherty, J. Sontowski, J. Moussafir, and J. Commanay, 2007: Micro-SWIFT-SPRAY presentation and validation cases. Chemical Biological Information Systems Conference and Exhibition. Austin, TX (USA), January 8-11, 2007.

Sontowski, J., C. Dougherty, J. Moussafir, G. Tinarelli, O. Oldrini, and E. Montanes, 2004: Evaluations of the Micro-SWIFT-SPRAY wind and transport-dispersion model for urban areas. Eighth Annual George Mason University, Fairfax, VA (USA), July 13-15, 2004.