H14-163
THE INDOOR / OUTDOOR POLLUTANT TRANSFER OF A HAZARDOUS RELEASE: APPLICATION TO A PARISIAN RAILWAY STATION

Maxime NIBART[1], Patrick ARMAND[2], Christophe OLRY[1], Christophe DUCHENNE[2] and Armand ALBERGEL[1]

[1] ARIA Technologies, F-92100 Boulogne-Billancourt, France
[2] CEA, DAM, DIF, F-91297 Arpajon, France

Abstract: In urban areas, a large part of the population is inside of buildings. In the case of a toxic or hazardous release, the two way transfer of material, infiltration and exfiltration, needs to be considered. Many urban models have been developed in the last few years but the coupling must be improved to answer questions as to the external effect of an indoor release and the consequences of an outdoor release on the internal environment of a large and crowded building. The present paper introduces the coupling between an urban dispersion model (MSS) and a CFD model (Code_Saturne) in order to accurately assess the relevant transfer effects. In particular, this work considers indoor releases that can occur in large semi-enclosed spaces such as railway stations. Different coupling methods are discussed. The selected method, which employs the nesting capability of a Lagrangian particle model and the wind fields from both MSS and Code_Saturne, is applied in the *Gare du Nord*, a Paris downtown area with several hypothetical meteorological conditions and releases. The contribution of the CFD flow assessment is clearly demonstrated.

Key words: *indoor-outdoor transfer, 3D Lagrangian dispersion model, 3D mass-consistent model, micro-scale, Code_Saturne, Micro-SWIFT-SPRAY, urban environment*

INTRODUCTION
Industrial accidents as well as 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 emergency preparedness and response. The challenge is to provide the most precise and reliable evaluation of the spatial and temporal distribution of the gases and/or airborne particles, in computation times consistent with the limited time frames of a crisis management situation. The Micro-SWIFT-SPRAY (MSS) modelling system developed by ARIA Technologies, ARIANET, MOKILI, and CEA is an intermediate quick response capability to simulate the micro-scale processes.

Infiltration of pollutants inside buildings is a key process in order to estimate health effects risks due to hazardous releases, especially in urban areas. Outdoor dispersion models like MSS (Moussafir *et al.*, 2010; Armand *et al.*, 2010) or the emergency response code ALOHA from US-EPA, compute the infiltration inside buildings with macroscopic methods, deriving analytical indoor concentrations from the outdoor concentrations. These methods are mainly based on an infiltration/exfiltration time scale that can be, in practice, complex to estimate. This time scale is linked with the building's air exchange rate which is the number of times per hour that the volume of air within the building is completely replaced by fresh air when doors and windows are closed. Moreover, in many accident situations (e.g. fires or malevolent actions), hazardous releases can occur indoor, in large semi-enclosed buildings, such as industrial facilities or public places (e.g. railway stations or institutional buildings) which are typically the kind of buildings with an infiltration time scale that is difficult to estimate and which might not even be relevant because of large openings.

To predict the atmospheric dispersion in detail and the sanitary consequences inside and outside, CFD models appear to be a possible solution. They are often used for both outdoor and indoor dispersion modelling. But the large calculation time of CFD is a significant disadvantage for operational application. Simpler but quicker models are often preferred. The system proposed here limits the use of CFD to the indoor domain. The outdoor dispersion is done by the short response model MSS, described below. However, a coupling method is required between MSS and the CFD model, Code_Saturne.

SHORT DESCRIPTION OF THE MODELS
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 and urban areas. Given topography, meteorological data and building geometry, 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 especially inside the flow zones modified by obstacles.
Micro-SPRAY is a Lagrangian particle dispersion model (LPDM) able to take into account the presence of obstacles. It is directly derived from the SPRAY code (Anfossi *et al*., 1998; Carvalho *et al*., 2002; Ferrero *et al*., 2001; Ferrero and Anfossi, 1998; Trini Castelli *et al*., 2003; Tinarelli *et al*., 1994 and 2000). It is based on a 3D form of the Langevin equation for the random velocity (Thomson, 1987).

The Code_Saturne model is the CFD model developed by EDF R&D (Archambeau *et al*., 2004). Its atmospheric version is developed at CEREA. The atmospheric dispersion is usually done with the RANS Eulerian capability of Code_Saturne. Yet a Lagrangian model is available in Code_Saturne and allows following real particles in a fluid, with turbulent dispersion and retro-action to fluid (dynamic and thermal). The dispersion of very small and passive particles with this Lagrangian model should allow the modelling of a passive gas. Some promising results have been obtained on wind tunnel comparison (case from CEDVAL database, Hamburg University).

COUPLING STRATEGIES

The coupling frame using two nested domains is defined as follows: the outer domain is performed with MSS doing only outdoor dispersion. The inner domain, mainly composed of indoor volumes, is performed with Code_Saturne. The pollutant transfer is from inside to outside and vice-versa.

Many strategies could be devised. The main key points which should be considered are: the dispersion in Code_Saturne can be Eulerian or Lagrangian; Code_Saturne could possibly be used only to compute wind fields; MSS is right now limited to structured mesh whereas Code_Saturne is compatible with unstructured mesh and so can more accurately consider complex geometries.

Inner and outer domains limits

Using CFD for the indoor dispersion could lead to the conclusion that the CFD domain should start at the doors, windows and others openings. But to perform an accurate indoor/outdoor pollutant transfer modelling, the interfaces should be computed with the best physics modelling available which is here the full Navier-Stokes equations set. So the limits of the inner domain are set a few meters away from the walls of the buildings where indoor flow is computed.

Wind coupling

A one way coupling has been implemented: the boundary conditions of Code_Saturne are driven by the 3D-output of Micro-SWIFT. Micro-SWIFT gives stationary fields of velocity, turbulent kinetic energy k and horizontal and vertical diffusivity coefficients K_z and K_h. These variables, characterizing an anisotropic turbulence, are converted and interpolated in time and space to set Dirichlet conditions for Code_Saturne used with the k-ε closure which characterizes an isotropic turbulence.

Taking advantage of the fact that the 3D results of Micro-SWIFT are easily available for Code_Saturne with this new development, the initialisation of Code_Saturne is done through an interpolation of Micro-SWIFT fields. This method can speed up the convergence of the CFD model and has already been used in the wind power energy field (Giebel *et al*., 2006).

Dispersion coupling

For the dispersion coupling, two methods have been selected. The first one could be named "nested Micro-SPRAY". The dispersion is done both in the inner and outer domain with the Micro-SPRAY LPD model. Code_Saturne is used only to compute wind and turbulence fields. Depending on their locations, the particles are moved in accordance with either the 3D field of Micro-SWIFT or that of Code_Saturne. This method mainly requires the development of nesting capabilities inside Micro-SPRAY and the export of Code_Saturne 3D results in a file format compatible with Micro-SPRAY. This method preserves some of the advantages of the MSS modelling system: as the 3 models are called in sequence (cf. **Σφάλμα! Το αρχείο προέλευσης της αναφοράς δεν βρέθηκε.**), several computation of pollutant dispersion can be done on the same wind case.

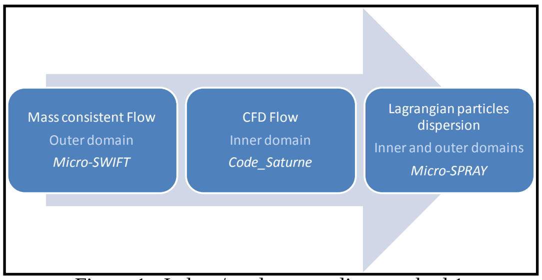


Figure 1 : Indoor/outdoor coupling: method 1

The second method involves Code_Saturne for an Eulerian dispersion. At each time step, Micro-SPRAY computes the dispersion in the outer domain and Code_Saturne computes the dynamics and the dispersion in the inner domain. This method requires the development of pollutant transfer algorithm between Micro-SPRAY and Code_Saturne. A Message Passing Interface (MPI) library, traditionally called in parallels programs, can be used to link the two models. This method allows keeping all the accuracy of CFD in the inner domain but would lead to larger computation times than method 1.

Most of the efforts described in this paper have been done using method 1.

Implementation of method 1

The coupling method 1 has been tested on single building cases. The pollutant transfer between the inner and outer domain has been checked and presents no mass loss. The best wind coupling is obtained with dimensions of the inner domain quite short (twice the dimension of the building) and with Dirichlet conditions at both inlet and outlet boundaries. If the boundaries of the inner domain are too far from the building, the deviations between Micro-SWIFT and Code_Saturne models can be significant and lead to a bad continuity of the flow across the frontier of the inner and outer domains.

The retro-action of Code_Saturne on Micro-SWIFT has not been implemented so far. Several iterations of retro-action between the two models could be a solution for a better continuity. But as Micro-SWIFT is based on an interpolation process without advection consideration yet, the effects of the retro-action could be too local to be significant.

APPLICATION TO GARE DU NORD, PARIS

The "nested Micro-SPRAY" method has been implemented centred on the area of *Gare du Nord*, Paris downtown. The outer domain is limited to an area of 900m by 900m but could have been the entire city since MSS has been parallelized (Duchenne *et al.*, 2011). The inner domain is an area of 385m by 385m.

The BD TOPO® database from IGN has been used to define the buildings, except for the railway station geometry that has been improved with observations (cf. Figure 2). The *Gare du Nord* railway station has 13 public doors with typical dimensions on its South facade and one very large opening on its North facade. The roof of the station is mainly composed of three large glass roofs.

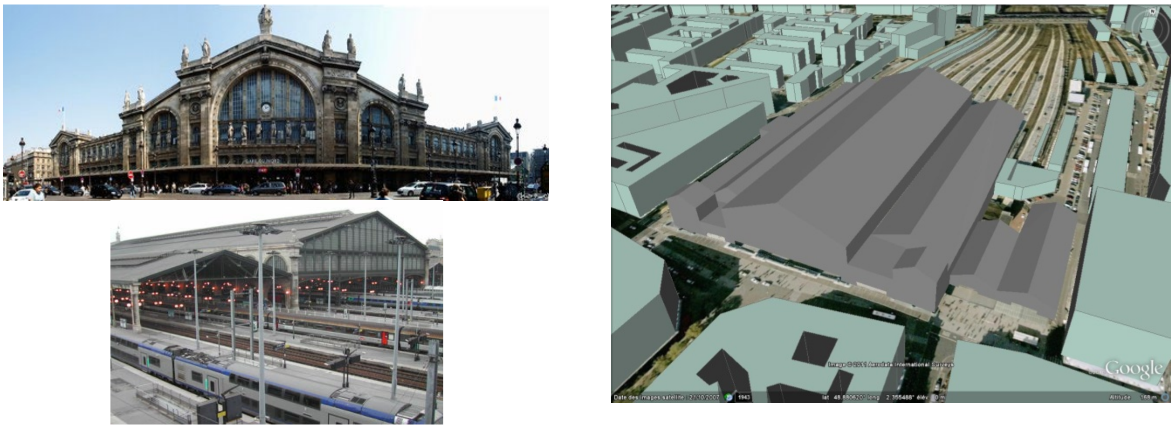


Figure 2. Pictures of *Gare du Nord* extracted from Google Earth - Views from South (left top) and North (left bottom) - *Gare du Nord* geometry and surrounding buildings from IGN BD TOPO® - View from South (right)

The two domains have been meshed with the same approach, projecting the buildings on a structured mesh. The horizontal resolutions of the two domains are respectively 3m and 1m. Figure 3 shows the buildings as considered by Code_Saturne (inner domain). Some indoor obstacles such as trains, pillar or kiosks that can be taken into account with a resolution of 1 m are included.

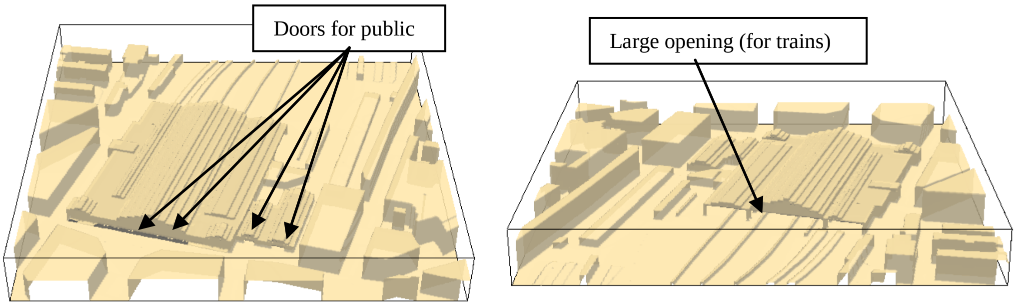


Figure 3. Inner domain - Code_Saturne mesh - View from South (left) and North (right)

Wind Fields

Two meteorological situations are presented here. They have the same velocity profile but with two distinct directions: West wind corresponding to low draft in the station and South wind corresponding to high draft in the station. All the boundaries conditions of Code_Saturne are Dirichlet type, both inlet and outlet conditions, using the method described previously. The two meteorological conditions are stationary in order to make the analysis easier but non-stationary conditions could have been performed. Figure 4 shows the flow near ground level in both the inner and outer domains. Good continuity is observed at the boundary between the two domains.

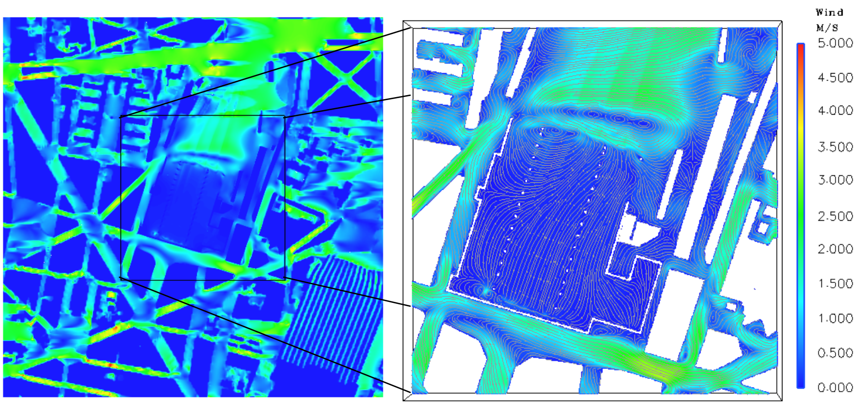


Figure 4. West wind – Wind velocity at 5 m above ground level – Outer and inner domain – (left) and Wind velocity and stream lines at 5 m above ground level – Inner domain (right)

Releases and dispersion

Two releases have been considered. They are both corresponding to the emission of a passive gas for 5 minutes with a mass flow rate of 0.5 $kg.s^{-1}$. The two releases differ only by their location: one is inside the rail station, and the other is outside. They are separated by 80 m. Their location can be seen on Figure 5 and Figure 6 (red concentration values). These figures show, exported in Google Earth, ground concentrations both in inner and outer domains. They illustrate the capabilities of the system to predict concentration fields inside the station and the indoor-outdoor transfer mechanism (both ways).

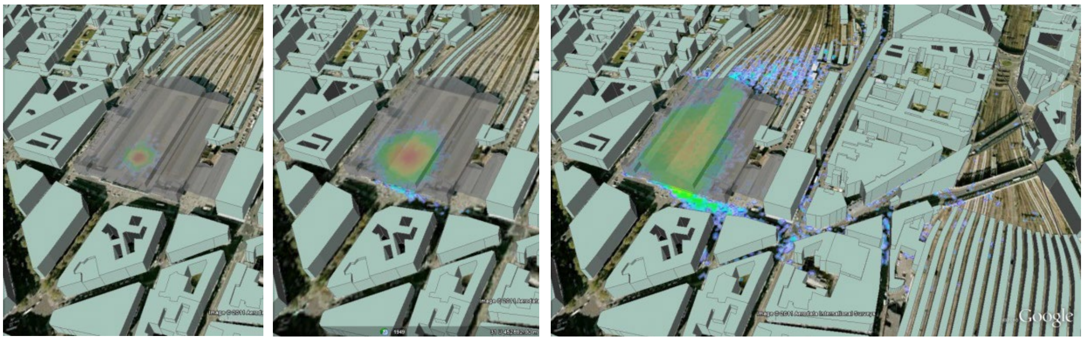


Figure 5. Ground concentration (indoor release – west wind) 2, 8 and 32 minutes after the beginning of the release

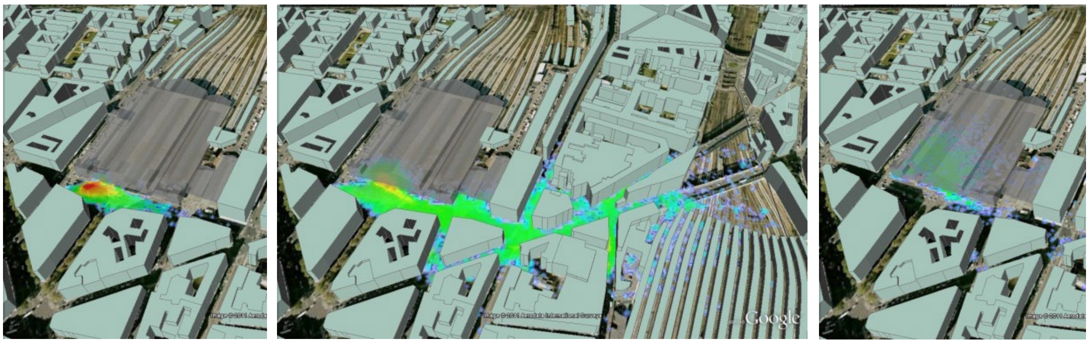


Figure 6. Ground concentration (outdoor release – west wind) 2, 8 and 32 minutes after the beginning of the release

Concentration time series at virtual sensors located far from the station and downstream of the releases have been extracted. They are plotted on Figure 7 and allow illustrating the global behaviour of the two releases highly depending on the wind direction. With a south wind, significant drafts are present is the station. The response time scales at the sensor location of indoor and outdoor releases dispersions (blue and red points) are very close. The peak concentrations are obtained at 10 and 15 minutes after the beginning of the emission. With a west wind, the response time scale of the indoor release is longer than the outdoor release. The outdoor release leads to a concentration peak 10 minutes after the beginning whereas the indoor release leads to a fairly constant level for more than 30 minutes. For both wind directions, the outdoor release has been also performed with standard MSS i.e. not considering the indoor/outdoor transfer mechanism (green points). No significant concentration is observed after 20 minutes. On the contrary, with the Code_Saturne coupling, significant concentrations (of same order of magnitude obtained with the indoor release) are computed after 30 minutes. These values are due to the portion of the pollutant which enters the station and then slowly leaks out.

Concentration time series at a point located inside the station have been also extracted (cf. Figure 8). The effects of the drafts are clearly observed: after one hour, the concentrations with south wind are much lower than with west wind. For south wind, the concentration peak is slightly higher with the outdoor release than with the indoor release. The chosen virtual sensor is actually closer from outdoor release plume axis than from indoor release plume axis.

These are preliminary observations and further analysis should lead to additional insight.

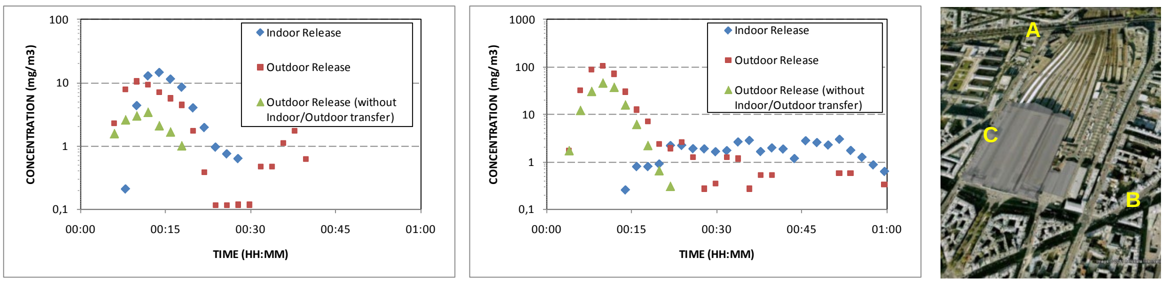
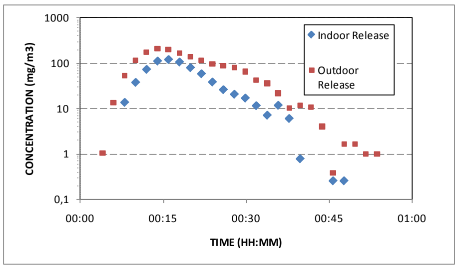


Figure 7. Temporal series of concentration at two downstream virtual sensors – Point A, *Bd de la Chapelle*, for South wind (left) and Point B, *Av de la Fayette*, for West wind (right)



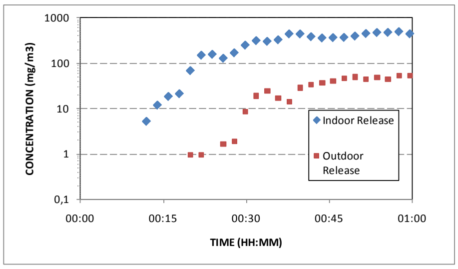


Figure 8. Temporal series of concentration at Point C inside the station – South wind (left) and West wind (right)

CONCLUSION AND PERSPECTIVES

The Micro-SWIFT-SPRAY modelling system has been coupled to the Code_Saturne CFD model in order to perform indoor/outdoor dispersion in an urban area near a large building. Application has been made to a railway station. Code_Saturne was used to compute flow inside the main building and its immediate environment. Micro-SPRAY performs the dispersion in both the inner and outer domains, using a nesting capability. Other coupling methods are possible but the calculation time and the use of one single model for the dispersion are the key points which led us to choose this specific approach.

The application of the method to the *Gare du Nord* station appears reasonable and consistent, though no measurements were available for comparison. The results appear to be a good proof of concept, illustrating the ability of the coupled system to compute the outdoor concentration due to an indoor release and the indoor 3D concentration field due to an indoor or outdoor release. The results show a significant dependency of the indoor/outdoor transfer time scale on the wind direction. This dependency is not taken into account in the existing infiltration model using a time scale (MSS or ALOHA) which concept is limited for such buildings with large openings leading to strong anisotropic infiltration/exfiltration. It would be interesting to perform validation against experimental measurements already available or from a dedicated campaign.

The coupling method conserves many of the advantages of the MSS modelling system. In an operational system running on a huge number of processors and covering an entire city with a downscaling from WRF or MM5 meso-scale models to MSS, Code_Saturne could be plugged as the indoor flow model for the smallest scale at some places of interest for a better consideration of indoor releases and a better assessment of the indoor contamination in some critical buildings.

REFERENCES

Archambeau, F., Mechitoua, N., Sakiz, M., 2004: Code Saturne: a finite volume method for the computation of turbulent incompressible flows, International Journal of Finite Volumes.

Anfossi D., F. Desiato, G. Tinarelli, G. Brusasca, E. Ferrero, D. Sacchetti (1998) "TRANSALP 1989 experimental campaignPart II: Simulation of a tracer experiment with Lagrangian particle models". *Atmospheric Environment*, **32**, 1157-1166

Armand P., C. Olry, J. Moussafir, A. Albergel and O. Oldrini, 2010 : Recent physical modelling developments in a lagrangian modelling system for emergency response purposes, Harmo13

Carvalho J., D.Anfossi, S. Trini Castelli, G. A. Degrazia (2002) "Application of a model system for the study of transport and diffusion in complex terrain to the TRACT experiment". *Atmospheric Environment*, **36**, 1147-1161

Duchenne C., P. Armand., O. Oldrini, C. Olry and J. Moussafir, 2011: Application of PMSS, the parallel version of MSS, to the micro-meteorological flow field and deleterious dispersion inside an extended simulation domain covering the whole Paris area, Harmo 14

Ferrero E., D.Anfossi (1998) "Comparison of PDFs, closures schemes and turbulence parameterizations in Lagrangian Stochastic Models". *Int. J. Environment and Pollution*, Vol. 9, 384-410

Ferrero E., Anfossi D. and Tinarelli G. (2001) "Simulations of Atmospheric Dispersion in an Urban Stable Boundary Layer". *Int. J. Environment and Pollution*, **16**, 1-6

Giebel G., G. Descombes, C. Lac, I. Marti Perez, A.Palomares, P. Louka, J. Badger, 2006: Short-term forecasting using advanced physical modeling , EWEC2006

Moussafir J., Oldrini O., Tinarelli G, Sontowski J, Dougherty C., (2004) A new operational approach to deal with dispersion around obstacles: the MSS (Micro-Swift-Spray) software suite. *Proc. 9th Int. Conf. on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes*, vol. 2, 114-118

Moussafir J., Buty D., Olry C., Nibart M., Albergel A., Tinarelli G., Anfossi D., Oldrini O., Harris T. and Dougherty C. (2007) SWIFT and MSS Current Developments. *11th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling*. Fairfax, VA (USA), July 10-12, 2007

Moussafir J., C. Olry, P. Castanier, G. Tinarelli , S. Perdriel, 2010: Applications of the mss (micro-swift-spray) model to long-term regulatory simulations of the impact of industrial plants, Harmo13

Thomson D.J. (1987) Criteria for the selection of stochastic models of particle trajectories in turbulent flows. *J. Fluid Mech*., Vol. 180, pp.529-556

Tinarelli G., Anfossi D., Brusasca G., Ferrero E., Giostra U., Morselli M.G., Moussafir J., Tampieri F. and Trombetti F., 1994: Lagrangian particle simulation of tracer dispersion in the lee of a schematic two-dimensional hill. Journal of Applied Meteorology, 33, N. 6, 744-756

Tinarelli G., Anfossi D., Bider M., Ferrero E.and Trini Castelli S. (2000) A new high performance version of the Lagrangian particle dispersion model SPRAY, some case studies. *Air Pollution Modelling and its Applications XIII*, S.E. Gryning and E. Batchvarova eds., Kluwer Academic / Plenum Press, New York, pp.499-507

Tinarelli G., Brusasca G., O.Oldrini, D.Anfossi, S.Trini Castelli, J.Moussafir (2007) "Micro-Swift-Spray (MSS) a new modelling system for the simulation of dispersion at microscale. General description and validation". Air Pollution Modelling and its Applications XVII, C. Borrego and A.N. Norman eds., Springer, 449-458

Trini Castelli S., Anfossi D., Ferrero E. (2003) "Evaluation of the environmental impact of two different heating scenarios in urban area". *Int. J. Environment and Pollution*, **20**, 207-217