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APPLICATIONS OF THE MSS MODEL (MICRO-SWIFT SPRAY) TO PHOTOCATALYTIC COATING SIMULATIONS

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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.
Photo-catalytic coating techniques (paint, cements) use the properties of TiO2 to produce a significant abatement of NOx in the vicinity of the surface where the coating is applied. An extended set of simulations was performed in cooperation between ARIA Technologies and ITALCEMENTI to examine the abatement performance in various urban situations, such as narrow streets or tunnels, when coating is applied on the ground or on facades or roofs, when traffic is moderate or strong.
These simulations have been validated both with field experiments and real world situations (Roma, Berlin). The ensemble of the simulation results have been cast into a library of results which users at ITALCEMENTI can use through a Web interface. This software tool, called EXP'AIR, is presented.

Key words: *Air quality simulation, photo-catalytic coating, building effects, Lagrangian dispersion modelling*

INTRODUCTION

Photo-catalytic coating techniques (paint, cements) use the properties of TiO2 to produce a significant abatement of NOx in the vicinity of the surface where the coating is applied. The numerical simulation of the NOx abatement efficiency of photo-catalytic coatings in urban environments requires the combination of three tools: (1) an emission model to represent the emissions from traffic, (2) a flow model allowing the simulation of small-scale urban flows influenced by buildings or tunnels, (3) a dispersion model to represent the dispersion and the deposition of the pollutant removed from the atmosphere by the photo-catalytic surfaces

The computation of NOx emissions from traffic is available through many computational tools using average emission factors, regularly updated as a function of the evolution of vehicles characteristics and fleet composition.

The flow and dispersion problem may be approached with fully-developed CFD models, using RANS or LES formulations, but their operation is delicate and requires extremely detailed information on buildings and refined meshes, because the constraints of the complete set of equations must be met. In the present work, we have applied a simplified approach, where a simplified diagnostic CFD model (Micro-SWIFT) is applied to obtain a mass-consistent representation of the flow, and a Lagrangian particle model (Micro-SPRAY) is used to compute the dispersion and deposition of NOx. The concatenation of these tools is called MSS (as Micro-SWIFT-SPRAY).

SHORT DESCRIPTION OF THE MSS MODEL (MICRO-SWIFT-SPRAY)

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 a 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).

DEPOSITION ALGORITHMS IN MICRO-SPRAY

The key improvements which were added to MSS for its application to photo-catalytic coating problems are the following:

- Generalization of the 3D meshes used in MSS to include anywhere full computational cells which are not ground-based. This is necessary to reproduce bridges, arches, tunnels and other important types of grids.
- Careful revision of the statistical deposition algorithm in order to introduce deposition on any surface in the 3D domain (ground, walls, roofs, ceilings under arches or tunnels). This involves combining the probabilities of deposition at ground and on the walls, computed as a function of distance from each surface.
- External parameterization of the type of surface for each facet of modelled buildings, in order to allow the use of specific deposition velocities at arbitrary places on the buildings (e.g.: facade, roof, for each floor)

PICADA VALIDATION

The validation work of MSS for applications to photo-catalytic coating was based on the PICADA Project (Photo-catalytic Innovative Coverings Applications for Depollution Assessment, an European Commission funded project with the objective to evaluate the depollution effectiveness of photo-catalytic coverings), which included small-scale field experiments managed by ITALCEMENTI on its Guerville research centre site. The experimental set up consisted of three consecutive street canyons with an aspect ratio of 0.4 (canyon width/height) made up of commercial cargo containers under a scale of 1:5 of an assumed street canyon length of ~100 m and consisting of seven storey buildings (~25 m). Each street has the approximate dimensions of 20 m length, 2 m width and 5 m height.

The selection of PICADA validation cases was made by choosing situations for which all/or almost all of the parameters necessary for the comparison measurement/model were at disposal (NOx concentration, meteorological parameters and emission data). Moreover, for each scenario, the meteorological conditions were chosen to be as identical as possible in order to enable the comparison between measurements in the TiO2 canyon and the Reference canyon. The model yields results with the same order of magnitude as found in the measurements. In the scenarios that best demonstrate the pollution abatement effect of the photo-catalytic coating, the efficiency of the TiO2 coating varies in the range 15% to 50% in the measurements and in the range 35% to 50% in the modelling simulations.

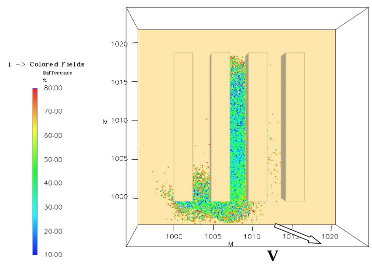
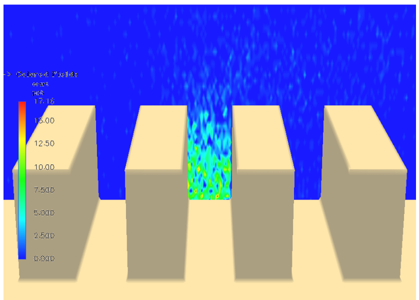
View from above (difference in %)	**Vertical cross section in the middle of the canyon (absolute difference)**
	

Figure 1: Example of MSS result for a reduction scenario. Difference (Reference-TiO2 canyon) in NOx concentration (ppb)

DESCRIPTION OF CONFIGURATIONS ANALYZED FOR EXP'AIR

The EXP'AIR system was designed to quickly show the abatement efficiency of photo-catalytic coating under different circumstances. Several geometric configurations were defined.

Street Canyon: The target of this configuration is to simulate a narrow street with relatively continuous façades in a typical European urban environment.

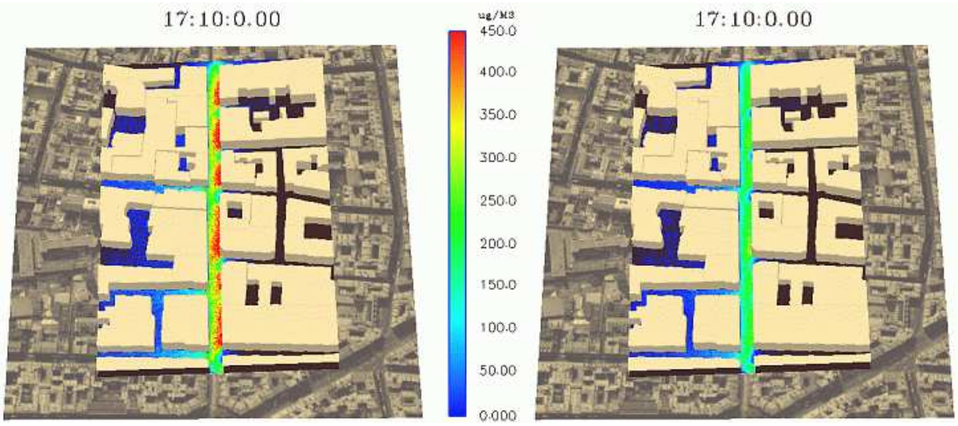


Figure 2: Illustration of the "Street Canyon" geometry (without TiO2 on the left, with TiO2 on the right).

Street without vis-a-vis: The facade configuration was simply created using the buildings on the left-hand side of the Street Canyon configuration.

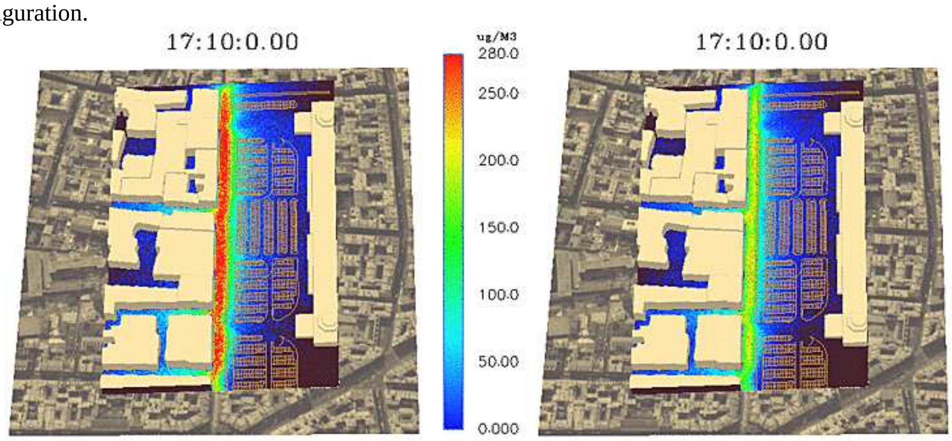


Figure 3: Illustration of the "Street without vis-a-vis" geometry (without TiO2 on the left, with TiO2 on the right).

Tunnel I/O: The Tunnel I/O configuration looks at the efficiency of photo-catalytic coating on the sides of access to tunnels.

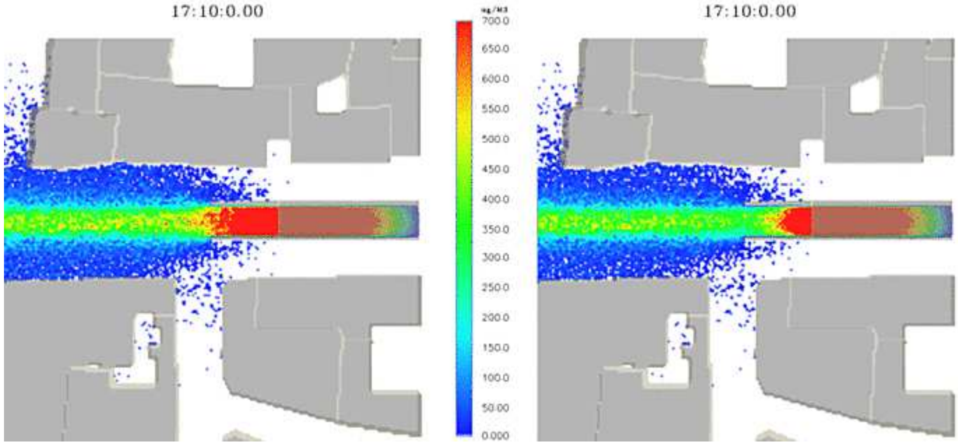


Figure 4: Illustration of the “Tunnel I/O” geometry (without TiO2 on the left, with TiO2 on the right).

Tunnel: The Tunnel configuration looks at the efficiency of photo-catalytic coating on tunnels of various lengths.

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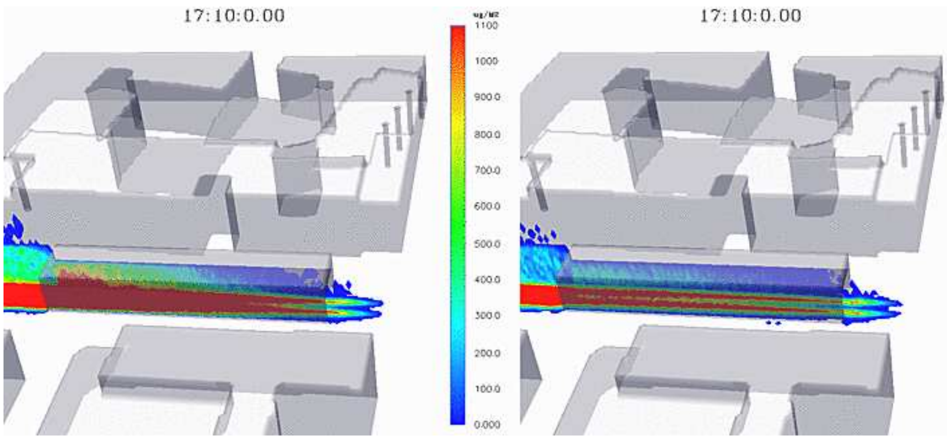

Figure 5: Illustration of the “Tunnel” geometry (without TiO2 on the left, with TiO2 on the right).

District study in Berlin: A realistic test case with a district in Berlin was simulated, taking into account emissions from traffic, domestic sources and isolated point sources. A snapshot of this type of simulation is presented in Figure 6.

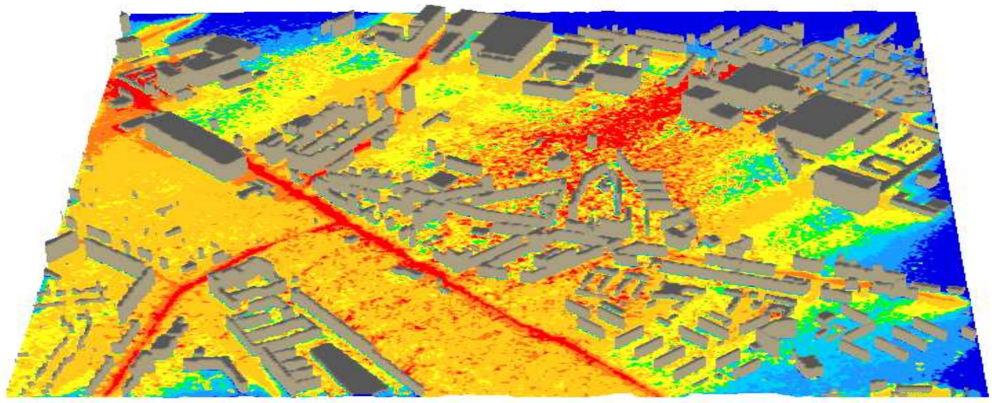

Figure 6: Snapshot of a realistic district simulation with MSS included into EXP’AIR (digital data for Berlin provided by WEST Sustainability and Virtual City Systems)

THE EXP’AIR SOFTWARE PACKAGE

The target of this joint work was to provide ITALCEMENTI personnel with a dynamic tool that could summarize the expected efficiency of various settings of photo-catalytic coatings. It was decided to avoid the complexity of submitting new runs, creating new computational meshes, running new simulations with no expert control. Hence the EXP’AIR tool was designed as a simple Web interface (html) to browse through a library of results. The results presented by EXP’AIR are comparative plots, charts and animations, evidencing the air quality improvement for the library of different cases. This very simple design has many key advantages: (1) it allows portability through several platforms without the need for the installation of external GIS or graphics packages: a Web browser is sufficient to view the results, (2) the translation work is made extremely simple and can be delegated to non-experts (French and English versions exist, Italian and Spanish versions are in process), (3) upgrades like the addition of new cases are quite straightforward, (4) addition of arbitrarily complex 3D videos and simulations is possible for new cases, and the graphs and videos can be created with any software tool.

Figure 7 is a snapshot of the second page of the EXP'AIR package, after the selection of language is made, and after the user has entered the "Streets and Tunnels" section. On the left-hand side of the screen, there is the selection of four menus: **Configuration**, **Wind direction**, **Level of Traffic**, **Depollution TX Aria.**
In the case shown, the options are as follows:

- The four **Configuration** options are: Street canyon, Street without vis-a-vis, Tunnel I/O, Tunnel.
- The two **Wind direction** options are: Parallel and Perpendicular (to the street).
- The two **Level of traffic** options are 200 vehicles/hour and 600 vehicles per hour.
- The various **Depollution by TX Aria** options are Facades (only), Roads (sidewalk only, roadway only), Roads + Facades.

By clicking on "start the simulation", the user triggers the display of two parallel animated plots showing the output close to the ground (1.5 m height) with and without the application of the photo-catalytic coating.

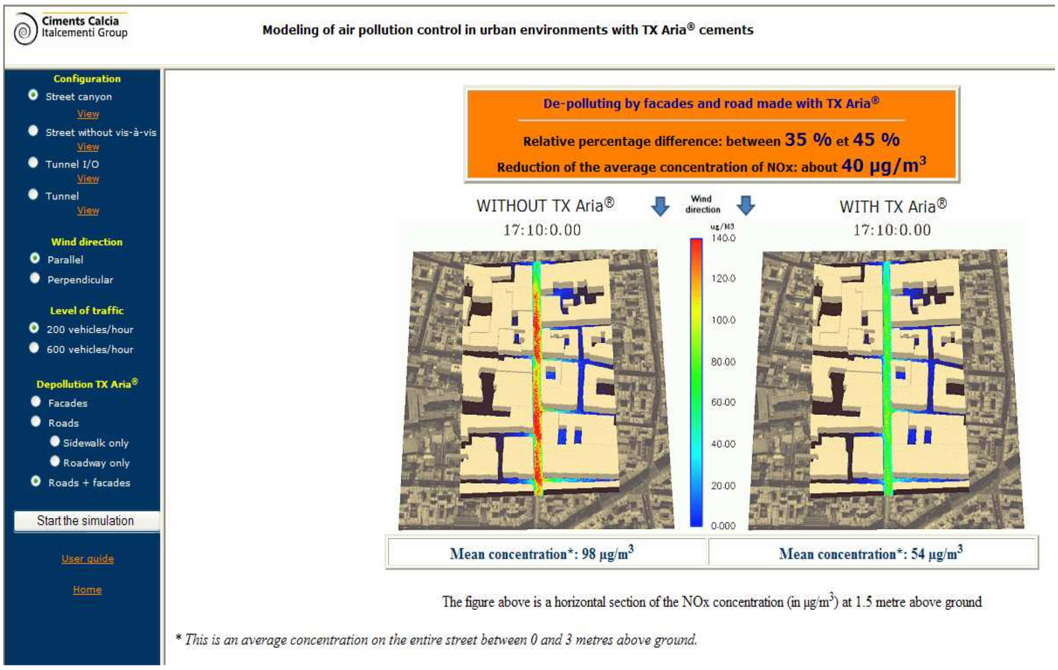

Figure 7: Snapshot of the working Web page of EXP'AIR. Selection of cases and controls are grouped on the left side of the page.

Menus are context sensitive, so that the different displays vary according to the cases. For the Berlin district case, as shown in Figure 8, concentration may be displayed at different heights (1.5m, 15m, 25m) to evidence the contribution of traffic and point sources at different heights.

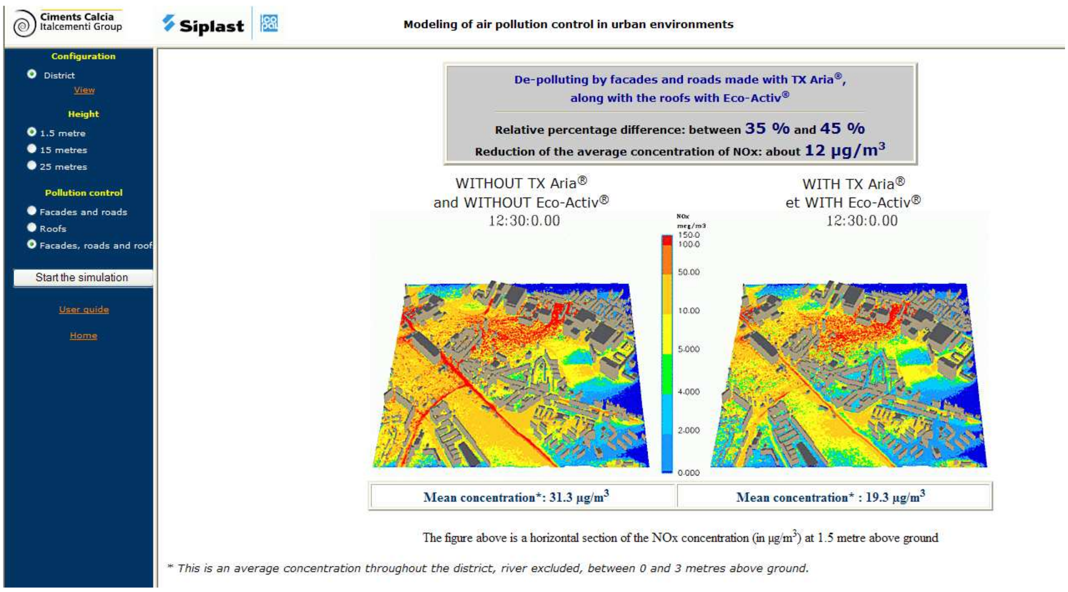

Figure 8: Snapshot of the working Web page of EXP'AIR Case of district scale Berlin simulation.

CONCLUSION

The MSS simulation system has been applied to a wide range of configurations, in order to simulate the abatement efficiency of TiO2 coatings. The results of this ensemble of simulations have been stored in a library of results accessible through a software package called EXP'AIR, which is now routinely used by ITALCEMENTI/Ciments Calcia in the preliminary discussions about the applicability of the photo-catalytic solutions. For the detailed definition of actual projects, specific runs of MSS are undertaken.

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