

COUPLING BETWEEN PMSS AND CONTAM: THE INDOOR / OUTDOOR CONTAMINANT TRANSFER OF A HAZARDOUS RELEASE

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Abstract: In the study of accidental or intentional releases of hazardous materials, modelling the evolution of contaminant concentrations using computational methods is increasingly used. Regarding on the scale and the environment considered for an outdoor urban area or an indoor multizone building, two different types of dispersion models are applied. Because contaminants can be released both outside and inside buildings, and can pass from one to the other, it is important to be able to model the exchange of contaminant between the two mathematical models. The main objective is to predict the ways outdoor air impacts on indoor air, and conversely, including the influence of atmospheric conditions and the building ventilation system. In this study, two different models are used: (i) for inside modelling, CONTAM developed by the NIST, a multizone airflow and contaminant transport analysis software, and (ii) for outside modelling, PMSS (Parallel-Micro-SWIFT-SPRAY developed by ARIA Technologies, MOKILI, and CEA), an association between a 3D wind field model for complex terrain (SWIFT) and a Lagrangian particle dispersion model (SPRAY) fitted for the urban pollutant dispersion. The proposed paper will present the tool we have developed which couples PMSS and CONTAM in a simplified two-way method and produces spatial and temporal 3D kml graphics for visualization of simulation results. In the coupling method, a first calculation of PMSS is performed in order to give the inlet conditions of contaminant concentrations and pressure-drop over time for CONTAM at flowpath links (PMSS2CONTAM part). Then CONTAM calculates the dispersal of airborne contaminants inside the building and return physical and temporal characteristics of sources that are re-emitting in the larger scale (CONTAM2PMSS part). We applied the tool for two cases of contaminant release in the urban area of Paris: (i) in a middle of the business district of La Defense considering a tower skyscraper and (ii) in a typical Parisian neighborhood considering a Haussmann building. The principal results will be displayed and commented on in the paper.

Key words: indoor-outdoor transfer, coupling, LPDM, CONTAM, SWIFT, SPRAY, urban environment

INTRODUCTION

In order to study as finely as possible the exposure of population on contaminant during the dispersion of a hazardous release in urban area, it is necessary to take into account interactions between indoor air and outdoor air. Indoor and outdoor domains represent two different scales and need to be considered by specific models. The present paper proposes the coupling of two models: (i) for the outdoor dispersion, the computation chain PMSS (Moussafir et al., 2010; Armand et al., 2010) which associates the meteorological model SWIFT and the dispersion Lagrangian particle model SPRAY in parallel versions and (ii) for the indoor, the multizone or nodes model CONTAM for contaminant dispersion inside the building.

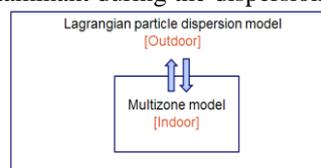


Figure 1: Indoor / Outdoor coupling

Compared to the simplified model for infiltration / exfiltration calculation already present in PMSS, the use of a multizone model such as CONTAM (Walton et al, 2005) allows to take into account the heterogeneity of flux at interfaces between indoor / outdoor, the differences between levels (floors) and to consider an emission source inside the building. Also the use of a multizone model allows keeping short calculation time compared to the use of a CFD model.

The main objective of this work is to predict the ways outdoor air impacts on indoor air, and conversely, including the influence of atmospheric conditions and building ventilation system.

We have developed two coupling tools, PMSS2CONTAM which downscale the dispersion from the urban area to the building area and CONTAM2PMSS which upscale the dispersion from the building area to the outside domain. These tools are embedded in a computation chain in order to perform a simplified two-way coupling in a non-iterative way. Finally, results of CONTAM can be visualized in Google Earth® (GE), thanks to a visualization tool called CONTAM2KML.

SHORT DESCRIPTION OF THE MODELS

The PMSS 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 (Anfossi D. *et al.* 1998). Micro-SPRAY (Tinarelli *et al.*, 2013) is a Lagrangian particle dispersion model (LPDM) able to take into account the presence of obstacles. It is based on a 3D form of the Langevin equation for the random velocity (Thomson, 1987).

CONTAM is a multizone software developed by the NIST and allows the calculation of airflows, delta P and contaminant transport between zones and across the envelope of a building based on a simplified macro-representation of the building.

PMSS2CONTAM

Micro-SWIFT and Micro-SPRAY supply on the outdoor domain two binary files (SWIFT.bin and SPRAY.bin) containing information of the 3D fields of the pressure differences (delta P) and the contaminant concentration. Starting from these files, the tool PMSS2CONTAM extracts these physical quantities at indoor / outdoor connection points of the envelope of the building in order to produce a WPC file. The WPC file is an input file for CONTAM containing the time series of delta P and contaminant concentration for all the airflow paths that are connected to the external environment. The location of these airflow paths are read from the PLD file (Path Location Data) which can be generated from the CONTAM GUI.

CONTAM2PMSS

CONTAM supply in a binary file (CONTAM.sim) results for each zone and each flow path connected to the external environment of source rejection position and temperature, contaminant release rate, height and diameter of sources. The tool CONTAM2PMSS post-treat the binary sim file in extracting these physical quantities in order to produce a PENTIM file which includes description of emission source terms for PMSS run.

CONTAM VISUALISATION TOOL

A KML file creation tool from CONTAM binary result file (CONTAM.sim) has been developed. This tool called CONTAM2KML allows visualizing in space and timing the concentration results of a CONTAM calculation in GE. Once the kml imported into GE, the user can select the level or the zone he wants to visualize.

By this way, it is possible to superpose 2D fields from PMSS results and 3D CONTAM results using CONTAM2KML in order to observe dispersion in the two different scale domains.

NON ITERATIVE TWO-WAY CHAIN

A calculation chain as a script shell invoking sequentially several executable and encapsulating PMSS2CONTAM, CONTAM2PMSS and CONTAM2KML has been developed. Feasible scenario for this chain corresponds to short time volumetric releases from the urban area. The results obtained take into account the outside dispersion of contaminants which infiltrate the building domain, and then, the exfiltration of these same contaminants after being dispersed by the multizone model from the inside to the outside. This chain defines a simplified two-way coupling because the invocation to the coupling tools is not iterative.

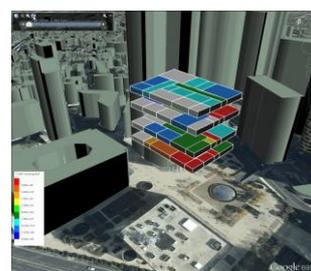


Figure 2: Example of GE visualization of CONTAM

VALIDATION CASE

We have carried out a validation case for the infiltration and exfiltration of the contaminant by comparing results of the coupling method with results of a reference ALOHA case of a 10 x 10 x 10 m building. Specifications of the validation case are displayed in table 1.

Table 1: Validation case specification

| Topo- graphy | Specie (m) | Source height (m) | Mass emitted (kg) | Meteo height (m) | Wind direction (degrees) | Wind speed (m/s) | Roughness (m) | Temp (°C) | Stability | air changes (s) |
|-----------------|---------------|-------------------------|-------------------------|------------------------|--------------------------------|------------------------|------------------|--------------|-----------|-----------------------|
| Flat | CO | 2 | 4 | 2 | 270 | 3.34 | 0.01 | 15 | Neutral | 60 |

The coupling method is sensitive to the definition of delta P in the envelope of the building. For this validation case we used a vertical and horizontal resolution of 1 m.

In Figure 3, on the left, are shown isocontours of CO concentrations at ground level computed by PMSS, on the right, the CONTAM sketchpad project we used for this case. The CONTAM project has been defined by a mechanical vent on the upwind face of the building in which the airflow pumped from the outside is imposed. On the opposite face, a natural opening for the exfiltration has been set. The value of the inflow debit has been derived from the building air exchange rate per hour and was 16.67 m³/s.

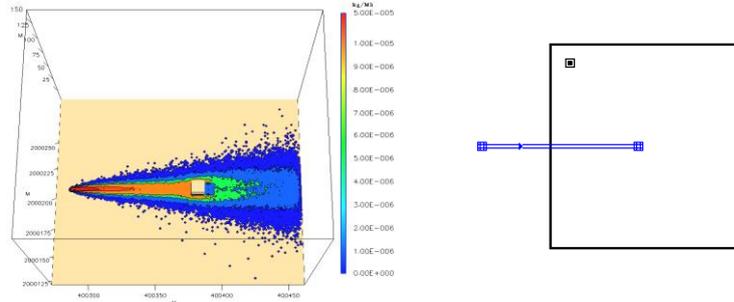


Figure 3: PMSS domain of validation case with CO ground concentrations in kg/m³ (left) and CONTAM sketchpad project (right)

Figure 4 shows comparison of indoor concentration results of CO in mg/m³ vs time in minutes between ALOHA (left) and the coupling method (right). We can see that there is a good correlation between the coupling tool and ALOHA (blue dashed curve).

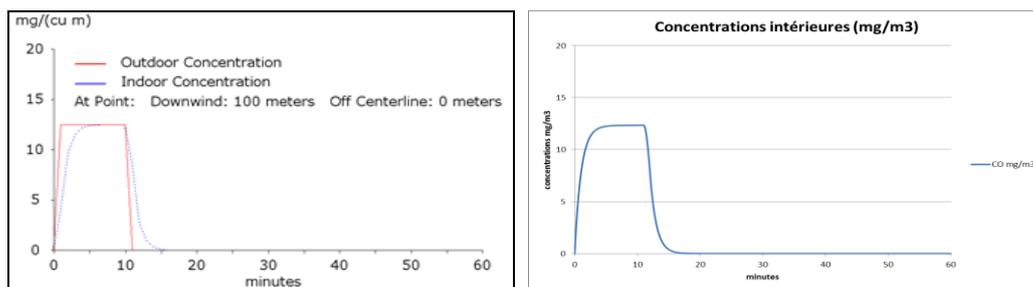


Figure 4 : indoor concentration comparison results between ALOHA (left) and the coupling method (right)

APPLICATION TO A SKYSCRAPER IN THE BUSINESS DISTRICT OF PARIS

In order to demonstrate the feasibility of computations using both CONTAM and PMSS in a more complex situation, we have carried out an application case to a tower in the middle of the business district of Paris using the two-way non iterative chain. The scenario modeled is as follow: A 5 minutes release of ⁶⁰Co impacting the tower which has 4 fictitious open windows at levels 20, 23, 27 and 30. The total duration of calculation is 120 minutes.

Table 2 shows specifications of the building used for the CONTAM project while Table 3 shows specifications of the PMSS domain.

Table 2: CONTAM building specification

| Lx (m) | Ly (m) | Lz (m) | Number of floors Type | Type of flow-path | External flow-path | Total floors |
|--------|--------|--------|-----------------------|-------------------|--------------------|--------------|
| 33.5 | 48.3 | 174 | 3 | natural | 4 | 52 |

Table 3: PMSS domain specification

| Lx (m) | Ly (m) | Lz (m) | Horizontal resolution (m) | Vertical resolution (m) | Vertical levels | Topography | Buildings |
|--------|--------|--------|---------------------------|-------------------------|-----------------|------------|-----------|
| 1050 | 900 | 500 | 6 | 2.5 at ground | 40 | yes | Complex |

In order that the outdoor release impacts the building, a south-east wind has been set for the first time frames. Meteorological conditions are neutral with a 2 m/s wind speed at 10m height. At the left of Figure 5, we can see a GE aerial view of the financial district and the tower modeled (in blue), at the center a Savi3D view of the part of PMSS domain where the ⁶⁰Co plume impacts the tower (black circle) and, at the right, a zoom of delta P and stream-lines around the building at 27th floor at the first calculation times.

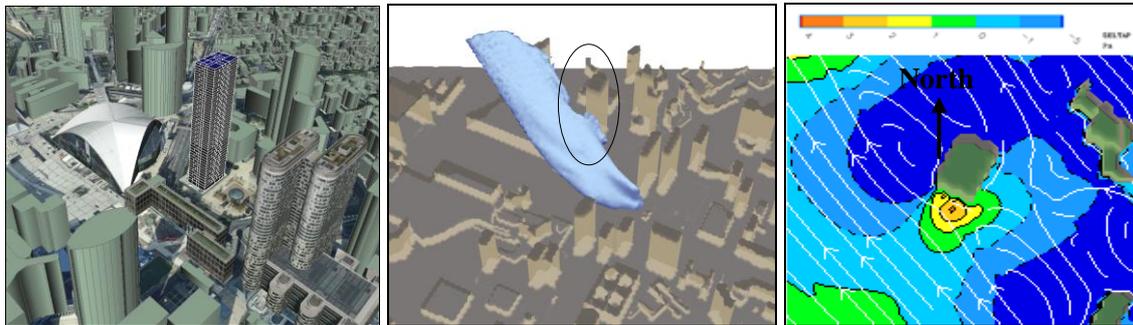


Figure 5: GE aerial view of the tower modeled (left); Savi3D view of the PMSS domain and CO60 plume impacting the tower (center); zoom of Delta P and stream-lines at 27th floor for the first calculation times (right)

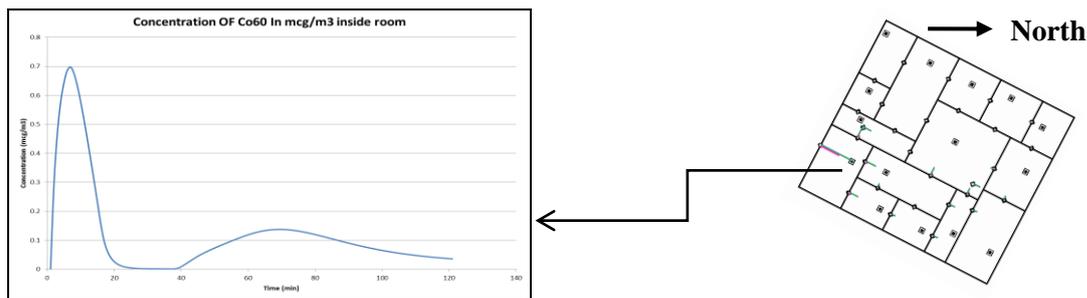


Figure 6 : ⁶⁰Co concentrations in mug/m³ vs time in min (left) of room indicated by the arrow from CONTAM Sketchpad result of the level 27 in which pink segments are delta P, and green segments are airflows

Figure 7 provides some results of ⁶⁰Co concentrations at level 27 for 3 time steps (2, 18 and 72 minutes). In Figure 6, at the right, the CONTAM sketchpad result for the first calculation times of level 27 and at the left, the graph of the evolution in time of Co60 concentrations inside the room indicated by the black arrow. As shown on the right picture of Figure 5, the connection path to the outdoor of the room observed is located at positive delta P. This means that during the passage of the plume at this level, as we can see on the left picture of Figure 7, there is an infiltration of ⁶⁰Co inside this room. This explains the first peak reached at about 5 minutes in the graph of Figure 6. On this graph we can also see a second peak between 40 and 100 minutes. This is due to the dispersion of contaminant inside the building. Indeed, the infiltration of ⁶⁰Co also occurs for level 20 in which another connection path to the outdoor has been

implemented. We can say that the ^{60}Co that infiltrated the building at level 20 took 40 minutes to reach level 27. On the two last pictures of Figure 7 (center and right), the plume has passed and the contours we see correspond to the interception of the 2D concentrations field of the exfiltration of the ^{60}Co that occurs at levels 23 (left side of the building, visible only on the right picture) and 30 (right side of the building).

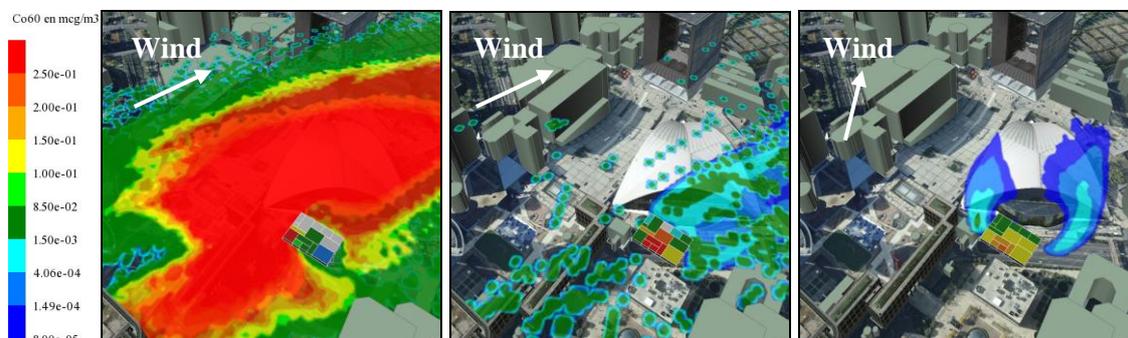


Figure 7: Combined 2D MSS and 3D CONTAM concentration results at level 27 for 3 time step, from left to right: 2, 18 and 72 minutes

CONCLUSION AND PERSPECTIVES

In order to realize contaminant dispersion simulation in both, urban area and inside the buildings, two coupling tools have been developed and the possibility to sequentially invoke them in a chain performing a non-iterative two-way calculation that takes into account both the influence of atmospheric conditions and the building ventilation system. The user can now visualize the CONTAM concentration dispersion in Google Earth® by using CONTAM2KML tool. The comparison results obtained for an academic case between the coupling method and the ALOHA model are satisfactory. Also, we have carried out an application for a tower in a business district in order to demonstrate the feasibility of PMSS / CONTAM computations in a complex built environment. This case has provided consistent and satisfactory results. For further development, it will be interesting to confront the results obtained with the coupled tools to a real case with observation data. Also the simplified two-way coupling is for the moment not iterative, it will be interesting to develop a complete two-way coupling that performs iterative calls of the tools.

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