DE LA RECHERCHE À L'INDUSTRIE

DEVELOPMENT AND APPLICATIONS OF RETRO-SPRAY

A BACKWARD ATMOSPHERIC TRANSPORT AND DISPERSION MODEL AT THE REGIONAL AND URBAN SCALES

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Harmo'15 Conference | Madrid (Spain) | 6-9 May 2013

Introduction – Motivation & Modelling system

- Industrial incidents as terrorist activities may result in noxious atmospheric dispersion
- In many situations (e.g. small leakage), it is not obvious that the magnitude of the release is enough to induce immediate and perceptible consequences on people
- However, it is often possible to detect even quite low concentrations of toxic substances
- It is thus necessary to determine the characteristics of the unknown source (ASAP)

- One solution is the "adjoint" transport equation method to compute backward propagation from detectors considered as sources and to identify the flied over areas
- As this functionality can be of great help in various risk and threat situations, it has been implemented it in the dispersion model SPRAY (ARIA Technologies, ARIANET and CEA)

- SPRAY is a LPDM dealing with 3D wind fields over complex terrains, able to take account of bounces and deposition on the buildings walls, and verifying a Langevin process with equations adapted to the local and regional scales inhomogeneous unsteady turbulence
- SPRAY is usually operated with SWIFT (3D diagnostic mass-consistent flow model)

Direct dispersion modelling in SPRAY

- In a LPDM, the motion of the numerical fluid particles verifies the relations:

  $du_i = a_i\, dt + b_{i,j}\, d\xi_j$ (1) and $dx_i = u_i\, dt = (U_i + u_i')\, dt$ (2)

  with $d\xi_j$ random increment of a Gaussian distribution, drift term a_i and random forcing $b_{i,j}$ obtained along Thomson (1987) theory with the main criterion of "well-mixed condition"

- In SPRAY, the horizontal velocity PDF is Gaussian and stationary whereas in convective atmosphere, the asymmetric and non-Gaussian vertical velocity PDF is represented by a Gram-Charlier PDF approximated by fourth order Hermitian polynomials

- From Wilson *et al.* (1983), Thomson (1987), and Carvalho *et al.* (2005):

  (i = x or y) $du_i = -(u_i / T_i)\, dt + 0.5\, (d\sigma_i^2 / dx_i)\, (1 + u_i^2 / \sigma_i^2)\, dt + (2\, \sigma_i^2 / T_i)^{1/2}\, d\xi_j$ (3)

  (i = z) $dw = (\sigma_w / T_w)\, (T_x / T_z)\, dt + \sigma_w\, (d\sigma_w / dz)\, (T_y / T_z)\, dt + (2\, \sigma_w^2 / T_w)^{1/2}\, d\xi_j$ (4)

  with σ_i the i^{th} velocity variance and T_i the i^{th} Lagrangian time

Carvalho, J.C. *et al.*, 2005: An iterative Langevin solution for contaminant dispersion simulation using the Gram-Charlier PDF. Environmental Modelling & Software 20, 285–289.
Thomson D. J. 1987: Criteria for the selection of stochastic models of particle trajectories in turbulent flows. *J. Fluid Mech*., **180**, 529–556.
Wilson J.D., B.J. Legg, and D.J. Thomson, 1983: Calculation of particle trajectories in the presence of a gradient in turbulent velocity variance, *Boundary Layer Meteorology*, **27**, 163-169.

Inverse dispersion modelling in SPRAY

- In inverse modeling (b like “backward” exponent), time is run through anti-chronologically in order to track back particles up to the source(s) leading to one or several detections

- Considering a positive time step (dt > 0), the previous relations readily become:

$$du_i^b = a_i^b\, dt + b_{i,j}^b\, d\xi_j \quad (1^b) \qquad \text{and} \qquad dx_i^b = -\, u_i^b\, dt = -\,(U_i^b + u_i'^b)\, dt \quad (2^b)$$

- According to Flesch *et al.* (1995) and Wilson *et al.* (2009), relations (3-4) transform into (3^b-4^b) where the change of sign in the drift acceleration may be noticed:

$$(i = x \text{ or } y) \qquad du_i^b = -\,(u_i^b / T_i)\, dt - 0.5\,(d\sigma_i^2 / dx_i)\,(1 + u_i^{b2} / \sigma_i^2)\, dt + (2\, \sigma_i^2 / T_i)^{1/2}\, d\xi_j \quad (3^b)$$

$$(i = z) \qquad dw^b = (\sigma_w / T_w)\,(T_x / T_z)\, dt + \sigma_w\,(d\sigma_w / dz)\,(T_y / T_z)\, dt + (2\, \sigma_w^2 / T_w)^{1/2}\, d\xi_j \quad (4^b)$$

Flesch T. K., J. D. Wilson, and E. Yee, 1995: Backward-time Lagrangian stochastic dispersion models and their application to estimate gaseous emissions.
Wilson J.D., E. Yee, N. Ek, and R. D’Amours, 2009: Lagrangian simulation of wind transport in the urban environment. Q. J. R. Meteorolog. Soc., 135, 1586-1602.

Implementation of Retro-SPRAY (1/2)

- Parametrization of a backward calculation requires limited changes *vs*. direct calculation:
  - Reversal of the initial and final times
  - Reverse use of the emission periods
  - Reverse storage of the concentration fields in the binary files
- (Retro-)SPRAY now reads multiple met'l files, each of them corresponding to unique time (SPRAY formerly designed to deal with chronological binary meteorological files)
- Retro-SPRAY uses the same 3D wind fields as SPRAY with :
  - Particles moved with (-U, -V, -W)
  - Signs of the velocity variances and Lagrangian time scales are unmodified
  - Vertical velocity PDF being asymmetric, P(-w) is considered instead of P(w)
- Retro-SPRAY as SPRAY are available in both scalar and parallel versions (parallelization by distributing particles to cores working on a unique or multiple tiles)

Implementation of Retro-SPRAY (2/2)

- Retro-SPRAY results are post-processed by a module called *Source_Detector*

1) For each sensor whose measurements $C_{mes}(t)$ are backtracked, release rate field is computed $Q(x_i,t) = C_{mes}(t) / C^*(x_i, t)$ where $C^*(x_i, t)$ is Retro-SPRAY retro-concentration field

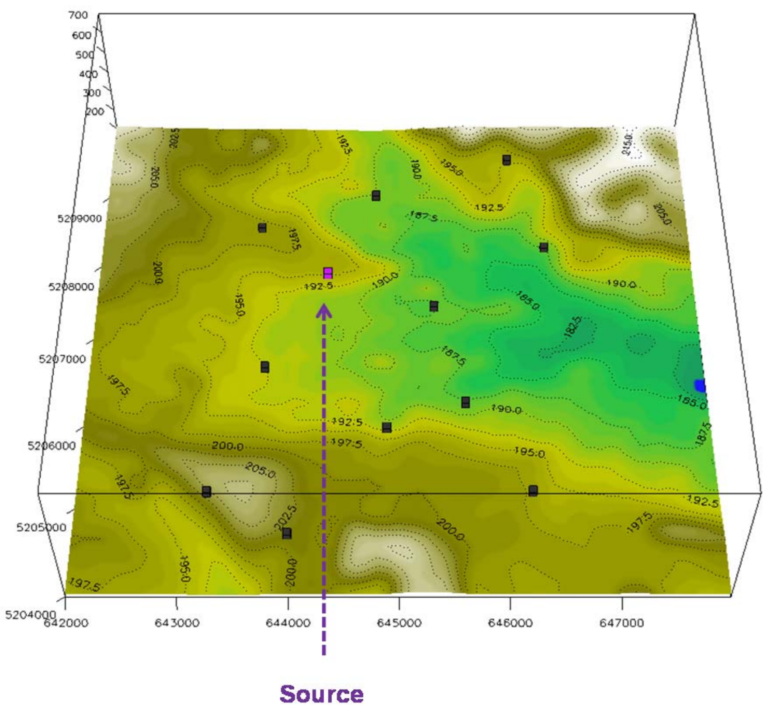
2) To avoid searching sources with unrealistic release rates, a threshold Q_{th} may be imposed (source region obtained taking into account met'l conditions and likely values of the release)

3) Once the release rate fields computed for each of the sensors Q_n ($n = 1\ldots N$) and $Q_n \leq Q_{th}$, overlapping between the Q_n fields is evaluated (integer in the interval $[0\ldots N]$)
(number of sensors measurements explained by a source at the considered point and time)

4) Sensors without measurement during all the time period may optionally be taken into account and the regions of the space with at least one "negative" (by convention) release rate subtracted

Test-case #1 – Presentation

- Case #1 is regional and representative of a facility in a rural or sparsely built environment which could be monitored either for the survey of its activities or to detect a possible incident (leakage…)
- Meteorological conditions:
  - Wind velocity of 4 m.s^{-1} at the source place; it turns gradually from N to NNE, and NNW – Stability class E
  - The wind field is characterized by its terrain following undulation with a weaker velocity in the valleys



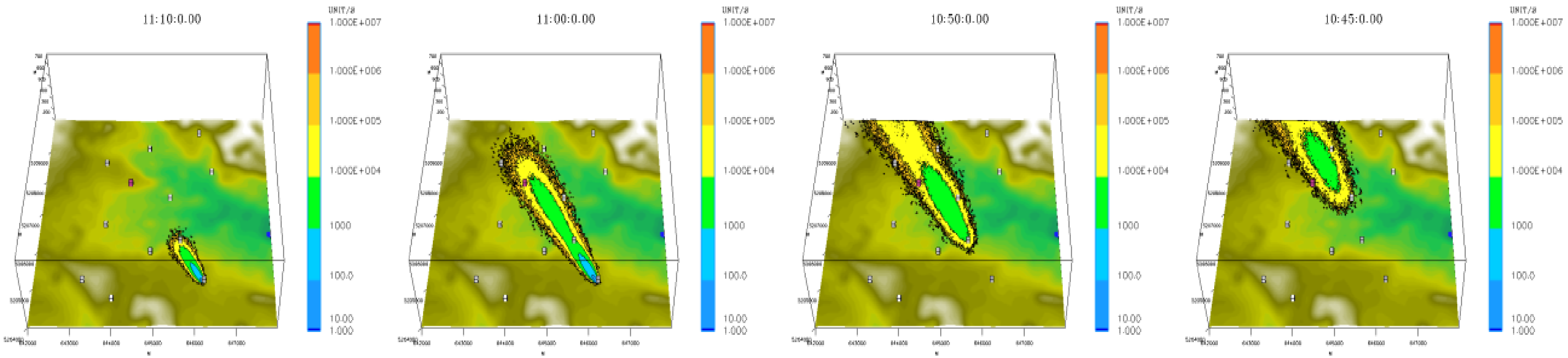
Source located on a real hilly terrain (Beaune, Burgundy, France) and surrounded by 11 sensors – Topography contour lines

Main conditions of the computation

Simulation domain	
Dimensions	6 km x 6 km
Number of meshes	300 x 300
Mesh size	20 m x 20 m
Releases	
Source height	10 m
Source dimensions	15 m x 15 m x 10 m
Time period #1	10:10 to 10:20
Rate #1	10^5 units.s^{-1}
Time period #2	10:50 to 11:00
Rate #2	10^5 units.s^{-1}
Detectors	
Height	10 m
Control volume	15 m x 15 m x 10 m
Average duration	5 min

Test-case #1 – Direct and inverse dispersion

- Direct dispersion simulation to evaluate the concentrations on the sensors
  - → *First and second releases switch on the detectors located resp. SW and SE of the source*
- Then, computations of retro-plumes from each of the sensors considered as retro-sources
  - → *36 periods of 5 minutes between 12:00 and 9:00 (if C_{mes} = 0, release = 0 ; if not, release = 1 / C_{mes})*
- Post-processing of the results to get the source release rate fields Q associated with each detector



Retro-history of the source release rate computed near the ground using SE detector #1 signal

The source is flown over by the retro-plume between 10:50 and 11:00. Release rate is in the colored area 10^4 – 10^5 units.s^{-1}

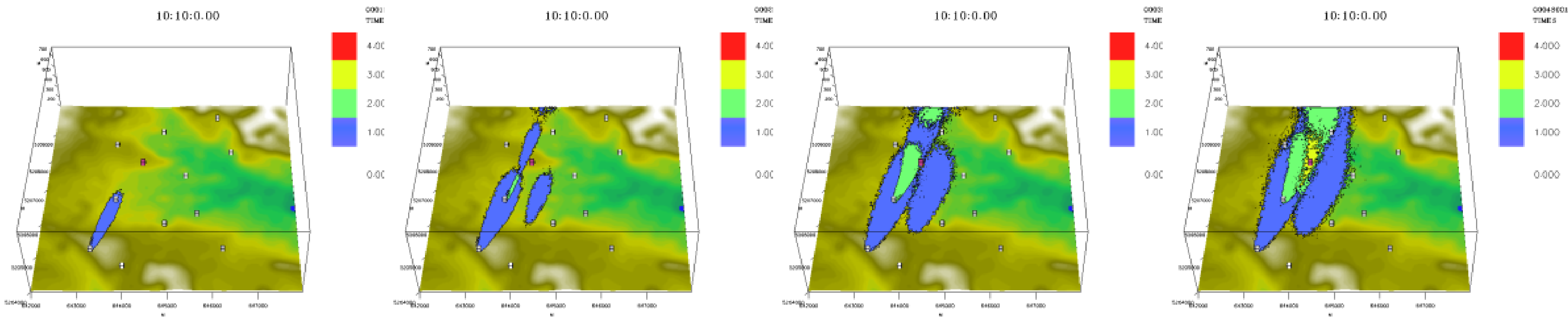
Actual release period #2 and source release rate in direct dispersion!

Test-case #1 – Overlapping of the release rates

- From the individual release rate fields, numbering of retro-plumes overlapping

  → *Release rate threshold Q_{th} from 10^3 to 10^8 units.s^{-1} – N.B. Highest number of detections is 3*

$Q_{th} = 10^3$ units.s^{-1} | $Q_{th} = 10^4$ units.s^{-1} | $Q_{th} = 10^5$ units.s^{-1} | $Q_{th} = 10^6$ units.s^{-1}



Number of retro-plumes overlapping for a source release rate maximum value of 10^3, 10^4, 10^5 or 10^6 units.s^{-1}

(section at 10 m AGL at time 10:10 of the release period #2)

If Q_{th} = 10^3 units.s^{-1}, the retro-plumes cannot reach the source location. For Q_{th} = 10^4 units.s^{-1}, the max. overlapping is 2.

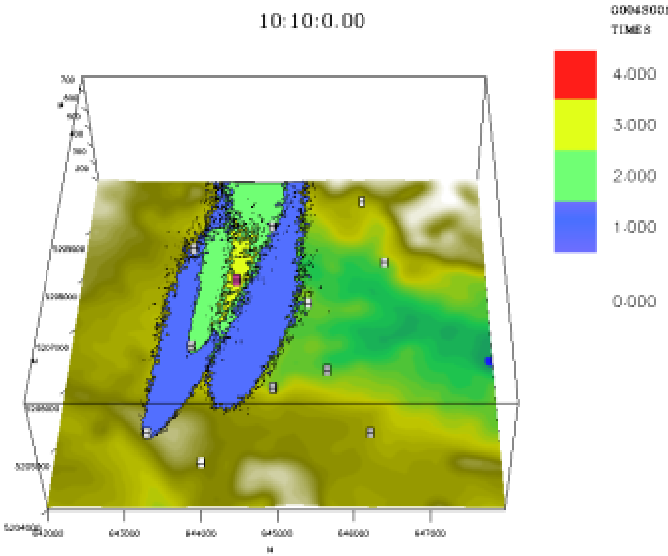
The highest number of detections is obtained for Q_{th} = 10^5 units.s^{-1}, the actual value of the release rate!

The area of the maximum overlapping corresponds to the source location!

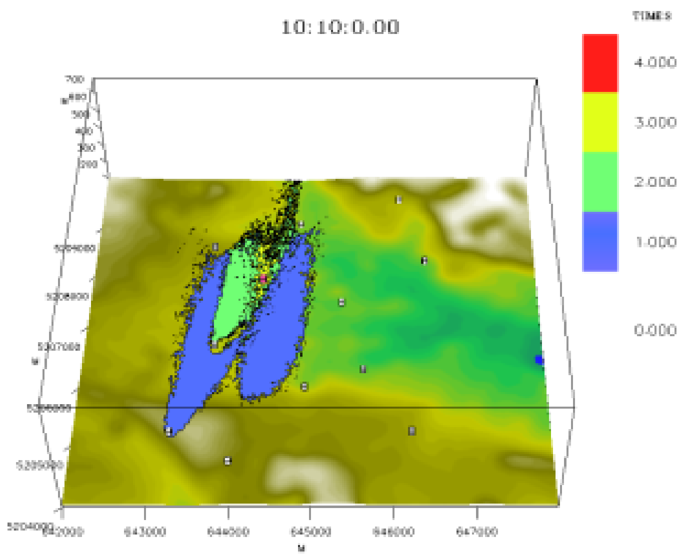
Test-case #1 – Taking account the “exclusions”

- Previous results ignore the “zero” measurements as the sensors measuring nothing in the time period
- Release rate fields can be computed from all of them and given a negative distinctive value
- Overlapping is then determined imposing a zero value at each point with a negative release rate

Without exclusion regions



With exclusion regions



Number of retro-plumes overlapping for a source release rate threshold value of 10^6 units.s^{-1}

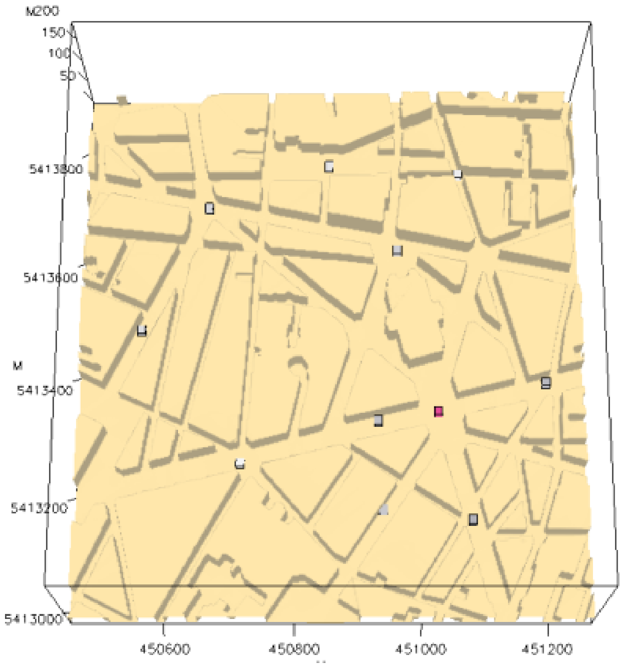
without (left) and with (right) consideration for the exclusion regions

(section at 10 m AGL at time 10:10 of the release period #2)

Subtracting areas prescribed by the “no-detections” refine the source characterization in terms of location and magnitude!

Test-case #2 – Presentation

- Case #2 is local and relevant to an accidental or intentional insidious toxic release in an urban area
- Meteorological conditions:
  - Wind is 3 m.s^{-1} at the source location; above the buildings, it turns from NE, to the S and NE – Stability class D
  - The wind field in the urban canopy is very complex and results from its orientation above the roofs, the channeling inside the streets network, and the influence of each building or group of buildings



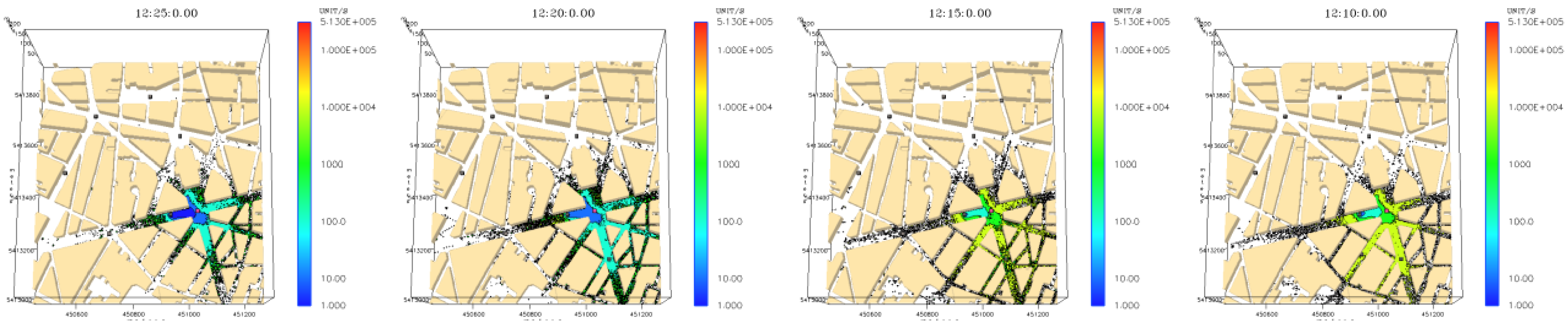
Places of the source and detectors – Buildings of the "Opera square" district in Paris where a brief emission is supposed to occur with 10 sensors arbitrarily set up

Main conditions of the computation

Simulation domain	
Dimensions	0.806 km x 0.880 km
Number of meshes	404 x 441
Mesh size	2 m x 2 m
Release	
Source height	2 m
Source dimensions	4 m x 4 m x 2 m
Time period	12:10 to 12:20
Rate	10^4 units.s^{-1}
Detectors	
Height	2 m
Control volume	4 m x 4 m x 2 m
Average duration	5 min

Test-case #2 – Direct and inverse dispersion

- Direct dispersion simulation to create a set of concentrations on the sensors
  - → *At each timeframe, the contaminant may be detected by a couple of sensors*
  - → *30 min after the beginning of the release, the species has totally disappeared from the domain*
- Then, computations of retro-plumes from each of the sensors considered as retro-sources
  - → *24 periods of 5 minutes from 13:00 to 11:00 (if C_{mes} = 0, release = 0 ; if not, release = 1 / C_{mes})*
- Post-processing of the results to get the source release rate fields Q associated with each detector



Retro-history of the source release rate in the streets network using detector #3 measurements

At 12:10, the retro-plume encompasses the source location and prescribes a release rate of 10^3 – 10^4 units.s^{-1}

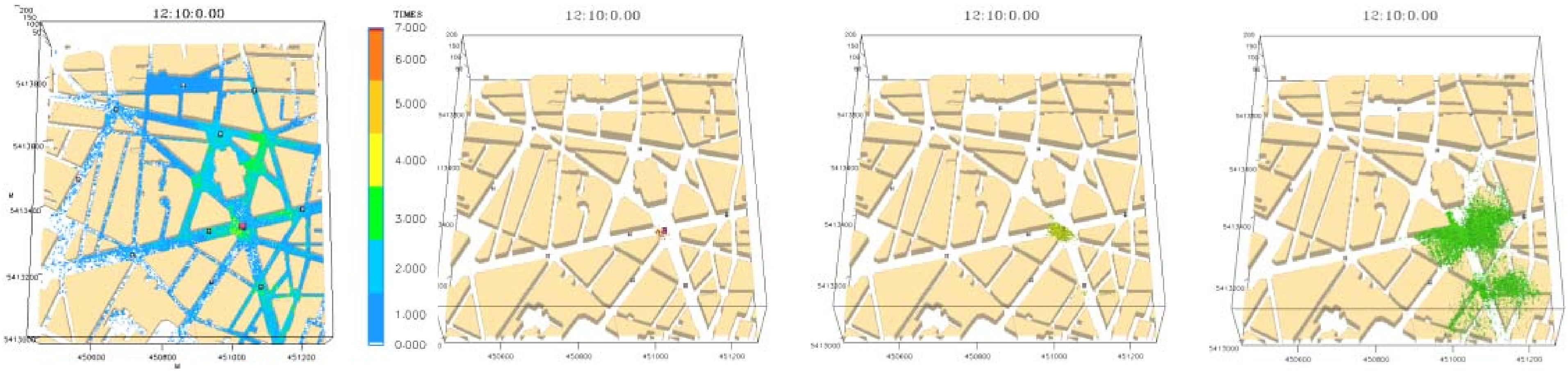
Actual time of the emission and release rate consistent with the real emission!

Test-case #2 – Overlapping of the release rates

- From the individual release rate fields, numbering of retro-plumes overlapping

  → *Release rate threshold Q_{th} from 10 to 10^6 units.s^{-1} – N.B. Highest number of detections is 7*

Section at 2 m AGL | 6 detections surface | 5 detections surface | 4 detections surface



2D section at 2 m AGL of the retro-plumes overlapping & 3D surfaces for a given number of detections

(all at time 12:10 for a source release rate threshold of 10^4 units.s^{-1}, i.e. the actual release rate)

Surfaces with 6 or 5 detections give a precise view on the source location!

Surface with 4 detections surface leads to a larger possible source region which stretches out along “Opera avenue”

For a max. release rate of 10^5 – 10^6 units.s^{-1}, even if the solution space expands, it still includes the real source location!

Conclusion & Perspectives

- Source Term Evaluation (STE) is a major issue for prevention, detection and intervention making use of measurements on pre-existing or set up in an emergency networks
- Retro-SPRAY has been developed as the “adjoint” (or inverse) model of SPRAY, LPDM fitting regional or local applications in simulation domains ranging 1 to 50 km
- Retro-concentration results are post-processed to identify possible source characteristics taking account of max. N# of retro-plumes overlapping and likely threshold release rate
- Retro-SPRAY has been validated in test-cases illustrating:
  - Routine survey of an industrial facility
  - Tracking of an insidious toxic release in a town district
- In all cases, Retro-SPRAY successful in back-tracking unambiguously sources (together, location, release rate and time) with a refinement when “non-detections” were also used
- Perspectives of this work:
  - Supplement first results with real wind tunnel or in-field noisy measurements (FFT 2007)
  - Use SPRAY combined with Bayesian approach including model and meas. uncertainties

Questions?

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