DEVELOPMENT AND APPLICATION OF RETRO-SPRAY, A BACKWARD ATMOSPHERIC TRANSPORT AND DISPERSION MODEL AT THE REGIONAL AND URBAN SCALE

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Abstract: The “adjoint” model of the SPRAY, a LPDM adapted to complex topography and built industrial or urban environment has been developed for Source Term Evaluation (STE) using the measurements issued by a network of sensors. “Retro-SPRAY” results are retro-concentration fields which are post-processed to determine the release rate fields leading to each individual detector signal, and the possible source region taking account of the retro-plumes overlapping and a physically sound release rate threshold. Retro-SPRAY and its post-processor have been validated at regional scale without obstacle, and at local scale in a built town district. The results give satisfactory utilizing non-zero measurements with a refinement in the STE if the “non-detections” are also considered. In a near future, this work will be supplemented with new tests of Retro-SPRAY using real wind tunnel or in-field noisy measurements.

Key-words: Retro-SPRAY, LPDM, backward transport, regional / local scale, scalar / parallel version.

INTRODUCTION

Both industrial incidents and malevolent or terrorist activities may result in the dispersion of noxious gases or particles in the atmosphere. In many situations (like a small leakage), it is not obvious that the magnitude of the release is enough to induce immediate and perceptible consequences on people in the vicinity of the event. However, for safety reasons, it is crucial and most often possible with appropriate sensors to detect even quite low concentrations of toxic substances. In case of such detection, it is thus necessary to determine the unknown location of the source, time of release, and release rate. One solution is to use the “adjoint” transport equation method. The principle is to compute backward propagation from detectors considered as sources and to identify the flied over areas which are possible locations for the release. As this functionality can be of great help in various risk and threat situations, it was decided to implement it in the dispersion model SPRAY, developed by ARIA Technologies, ARIANET and CEA.
SPRAY is a LPDM dealing with 3D wind fields over complex terrains, also able to take account of bounces and deposition on the buildings walls. It verifies a Langevin process using equations specifically adapted to the local and regional scales inhomogeneous and unsteady turbulence. SPRAY is usually operated with SWIFT, a 3D diagnostic mass-consistent flow model adapted to the built environments.
This paper aims at presenting Retro-SPRAY the backward transport model recently developed in SPRAY and associated test-cases in various atmospheric environments.

DIRECT AND INVERSE DISPERSION MODELLING

In a LPDM, the motion of the numerical fluid particles is defined by the generalized Langevin equations and verifies the relations:

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

With $x_i = (x, y, z)$ and $u_i = (u, v, w)$ the coordinates and velocity components of the particle, a_i and $b_{i,j}$ functions of (x_i, u_i, t), $d\xi_j$ a random increment of a Gaussian distribution (mean = 0 and variance = dt), and U_i and u_i' the average and fluctuating wind. The drift term a_i and the random forcing $b_{i,j}$ are obtained along Thomson (1987) theory with the main criterion of “well-mixed condition” to be respected.
In SPRAY, the horizontal velocity probability density function (PDF) is supposed to be Gaussian and stationary whereas in a 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), equation (1) becomes for horizontal (i = x or y) and vertical (i = z) components (with σ_i the i^{th} velocity variance and T_i the i^{th} Lagrangian time):

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

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

In inverse modeling (designated afterwards by the 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:

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

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:

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

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

IMPLEMENTATION OF THE INVERSE MODELLING IN PSPRAY

In Retro-SPRAY, the parametrization of a backward calculation requires limited changes compared to a direct calculation: reversal of the initial and final times, reverse use of the emission periods, and reverse storage of the concentration fields in the binary files. As SPRAY was designed to deal with chronological meteorological files (which is not convenient for inverse simulations), the model was optimized in order to read multiple binary files, each of them corresponding to a unique time.
Otherwise, Retro-SPRAY uses the same 3D wind fields as SPRAY with the difference that the particles are moved with (-U, -V, -W). Signs of the velocity variances and Lagrangian time scales are unmodified while the 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, as the changes between direct and backward modelling do not interact with the model parallelization which is performed by distributing particles to computer cores working on a unique tile or on multiple tiles.

SOURCE_DETECTOR POST-PROCESSOR

The *Source_Detector* module has been specifically developed for Retro-SPRAY results post-processing.
(1) For each of the sensors whose measurements are backtracked, *Source_Detector* computes the release rate field $Q(x_i,t) = C_{mes}(t) / C^*(x_i, t)$ where $C_{mes}(t)$ is the times series of the concentrations recorded by the detector and $C^*(x_i, t)$ is the retro-concentration field issued by Retro-SPRAY.
(2) Of course, Q increases with the distance from the detector. To avoid searching sources with unrealistic release rates, a threshold for Q, denoted by Q_{th}, may be imposed by the user (depending on the expected or likely range of source emission). Thus the possible source region is obtained for each sensor signal taking into account both meteorological conditions and physical values of the release.
(3) Numbering the sensors, the post-processor delivers all the associated release rate fields Q_n (n = 1…N) and $Q_n \leq Q_{th}$. Then *Source_Detector* determines the overlapping between the Q_n fields and returns a field of integers in the interval [0…N] corresponding to the number of sensors measurements which can be explained by a source emitting at the considered point and time at a release rate less than Q_t.
(4) Sensors without measurement during all the time period may optionally be taken into account. From them, release rate fields are simulated and artificially given a negative value. The same process as before is then applied considering a threshold release rate and subtracting the regions of the space where at least one negative release rate is encountered.

TEST-CASE #1 – REGIONAL SCALE AND COMPLEX TOPOGRAPHY

Presentation of the test-case

This first case is relevant to a facility in a rural or sparsely built environment which could be monitored either for a survey of its activities or to detect a possible incident (like a leakage). Figure 1 presents the source which is located on a real hilly terrain and surrounded by 11 sensors. The main properties of the simulation are summarized in Table 1. The wind has a constant velocity of 4 $m.s^{-1}$ at the source place. It turns gradually from N to NNE, and NNW. The stability class is E. The wind field is characterized by its terrain following undulation with a weaker velocity in the valleys.

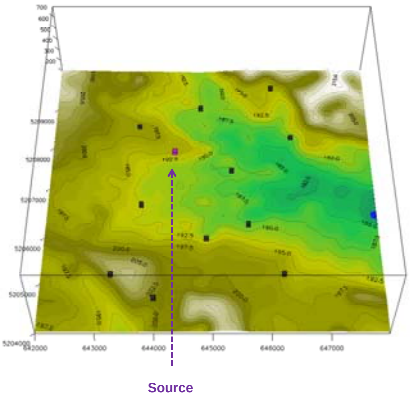

Figure 1: Case #1 – Places of the source and detectors. Topography contour lines.

Table 1: Case #1 – 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

Direct and inverse dispersion modelling

First, a direct dispersion simulation is carried out to evaluate the concentrations on the sensors. The first and second releases (see Table 1) switch on the detectors located respectively SW and SE of the source. Then, retro-plumes are computed from each of the sensors which are considered as retro-sources emitting during 36 periods of 5 minutes between 12:00 and 9:00 (if the concentration C_{mes} measured during the period is nought, the release is zero; if not, it is 1 / C_{mes}). Finally, Retro-SPRAY results are post-processed to get the source release rate fields Q associated with each detector. Figure 2 illustrates the first vertical level section of the release rate field evaluated with the SE detector #1 measurements. Between 10:50 and 11:00 (release period #2), the source is flown over by the retro-plume. Moreover, it is in the colored area where the release rate is $10^4 – 10^5$ units.s^{-1} which is the actual source release rate in the direct dispersion.

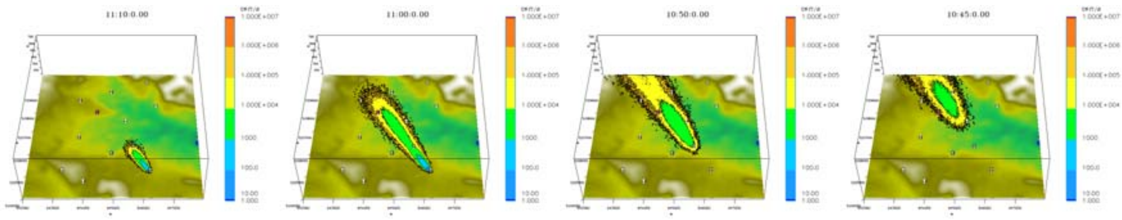

Figure 2: Case #1 – Evolution of the source release rate computed near the ground using SE detector #1 signal.

Overlapping of the release rate fields

From the individual release rate fields, the retro-plumes overlapping are numbered considering a release rate threshold from 10^3 to 10^8 units.s^{-1}. Note that in test-case #1, the highest number of detections is 3. Figure 3 shows the section at 10 m AGL of the overlapping number at 10:10 for a maximum release rate Q_{th}. If $Q_{th} = 10^3$ units.s^{-1}, the retro-plumes cannot reach the source location whereas for $Q_{th} = 10^4$ units.s^{-1}, the maximum number of overlapping is 2. The highest number of detections is obtained for $Q_{th} = 10^5$ units.s^{-1} (or more), the same value as the actual release rate. Moreover, the source is located in the area of the maximum overlapping. The same excellent result is obtained with the release at 10:50 which proves Retro-SPRAY ability to find back together the location, release rate and release time of the source.

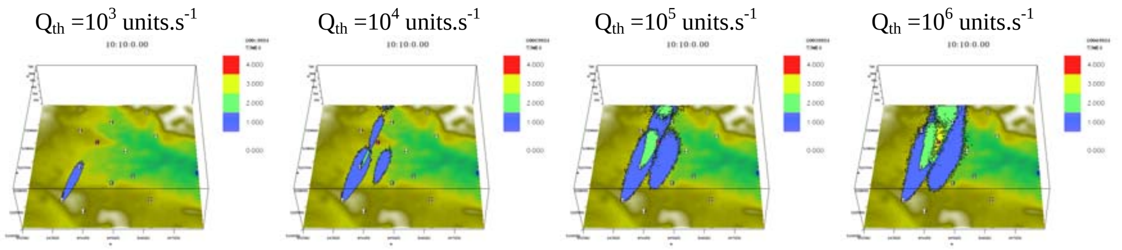

Figure 3: Case #1 – Numbering of the release rate retro-plumes overlapping for a source release rate maximum value of 10^3, 10^4, 10^5 or 10^6 units.s^{-1}.

Seeking for source term taking account of "exclusion regions"

The previous results ignore the nought measurements as the detectors which measure nothing during the whole time period. However, release rate fields can be computed from all of them and given a negative distinctive value. The overlapping is determined as before but imposing a zero value at each point with a negative release rate. Figure 4 presents the same results as Figure 3 for a release rate threshold $Q_{th} = 10^6$ units.s^{-1} using or not "exclusions". It appears that subtracting areas prescribed by nought measurements supplements the information and refine the source characterization in terms of location and magnitude.

Without exclusion regions | With exclusion regions

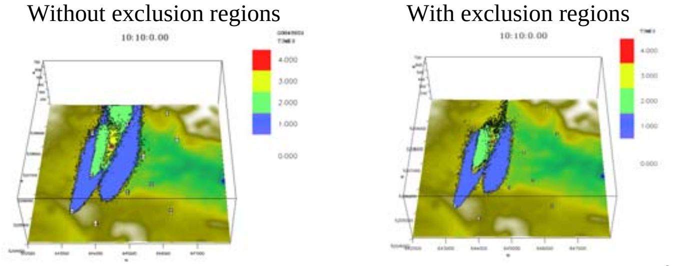

Figure 4: Case #1 – Same of Figure 3 for a release rate maximum value of 10^6 units.s^{-1} without (left) and with (right) consideration for the exclusion regions.

TEST-CASE #2 – LOCAL SCALE AND DENSELY BUILT ENVIRONMENT

Presentation of the test-case

This second case may correspond to an accidental or intentional insidious toxic release. It is very different from the first case as the scale is local and the release situated in an urban area. Figure 2 shows the district of the "Opera square" in Paris where a brief emission is supposed to occur with 10 sensors arbitrarily set up. The principal properties of the simulation are gathered in Table 2. The wind is 3 m.s^{-1} at the source location. Above the buildings, the wind blows from the SW, then turns to the S and the NE. The stability class is D. The wind field in the urban canopy results from its orientation above the roofs, the channeling inside the streets network, and the influence of each building or group of buildings.

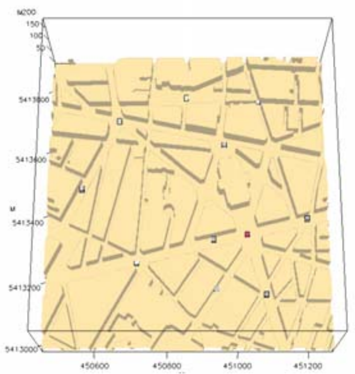

Figure 5: Case #2 – Places of the source and detectors. Buildings of the Opera square district (Paris).

Table 2: Case #2 – 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

Direct and inverse dispersion modelling

As in case #1, a direct dispersion simulation is performed to create a set of concentrations on the sensors showing that at each timeframe, the contaminant may be detected by a couple of sensors. Thirty minutes after the beginning of the release, the emitted species has totally disappeared from the simulation domain. Then, retro-plumes are computed from each sensor emitting during 24 periods of 5 minutes from 13:00 to 11:00 and Retro-SPRAY results are post-processed to have the source release rate field for each detector.

Figure 6 presents the first vertical level section of the release rate field estimated with the detector #3 signal. At 12:10 which is the actual time of the emission, the retro-plume encompasses the location of the source and prescribes a release rate at that place of 10^3 – 10^4 units.s^{-1} consistent with the real emission.

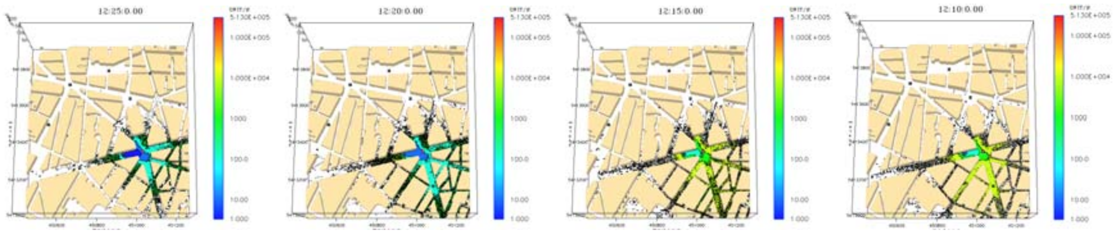

Figure 6: Case #2 – Evolution of the release rate in the streets network making use of detector #3 measurements.

Overlapping of the release rate fields

Exploiting the release rate fields, the retro-plumes overlapping are numbered with a release rate threshold from 10 to 10^6 units.s^{-1}. In test-case #2, the highest number of detections is 7. Figure 7 shows the section at 2 m AGL of the overlapping and the surfaces for a given number of detections, both at 12:10 and for a threshold value $Q_{th} = 10^4$ units.s^{-1} which is the actual release rate. The surfaces with 6 or 5 detections give a precise view on the source location while 4 detections surface leads to a larger possible source region which stretches out along "Opera avenue" meaning that a source in this street or over the roofs could also explain the measurements on the sensors. However, for a maximum release rate of 10^5 – 10^6 units.s^{-1}, even if the solution space expands, it still includes the real source location.

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

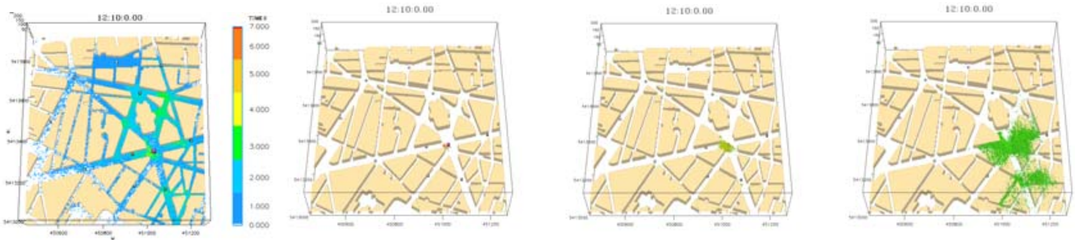

Figure 7: Case #2 – Numbering of the release rate retro-plumes overlapping
and 3D views of the surfaces with 6, 5, or 4 detections for a release rate threshold of 10^4 units.s^{-1}.

CONCLUSION

In case of potentially noxious atmospheric releases, the Source Term Evaluation (STE) is a major issue together for prevention, detection and intervention. The principle is to make use of measurements on pre-existing or set up in an emergency networks to try and determine the location, magnitude and / or kinetics of the source term. To fulfill this aim, Retro-SPRAY has been developed as the adjoint (or inverse) model of SPRAY, a LPDM fitting regional or local applications in simulation domains ranging from 1 to 50 km. Retro-SPRAY results consist in retro-concentration fields with are post-processed to identify the possible location of the source leading to detections taking into account the maximum number of retro-plumes overlapping and a likely threshold release rate. Retro-SPRAY has been validated in test-cases illustrating the routine survey of an industrial facility and the tracking of an insidious toxic release in a town district. First, fictitious measurements were produced by direct dispersion simulations. Then, STE were triggered with the artificial detections. In all cases, Retro-SPRAY was successful in back-tracking unambiguously sources especially when "non-detections" were also used. Perspectives of this work will be to supplement these first results with real wind tunnel or in-field noisy measurements, like e.g. the FFT 2007, and to use Retro-SPRAY combined with Bayesian approaches including modelling and measurements uncertainties.

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