Response to the Reviewer #1

The idea of the paper is to achieve the best result with as less as possible information. This idea is very innovative and I support any new effort. The application is the atmospheric dispersion in urban areas. The goal is to find the source when we know the flow field and the real concentration measurements.

I have one major comment/question.

When authors try to validate this approach they compare results of source inversion (distance to true source etc) with 'optimal network' of 10 sensors with the results obtained by the full network (40 sensors). Why don't they directly compare results of 'optimal' network of 10 sensors with the results of other networks of 10 sensors? Of course, there are too many of such networks. But by application of the combination same procedure as we did in Kovalets et al (2011) and Efthimiou et al (2017) they at least could prove that their 'optimal network' yields the results within say best 5 or 10% of the results that could be achieved with 10 sensors.

Reply: *We would like to thank Dr. Efthimiou for the positive feedback and we appreciate his comments/questions. We have carefully considered his comments and worked to include them in a revised version of the manuscript according to the proposed suggestions.*

Dr. Efthimiou's above comment can be complied into two following comments and please find below the responses to these as follows:

Comment 1: Why don't we directly compare results of the 'optimal' network of 10 sensors with the results of other networks of 10 sensors?

Reply: *The comparison with networks of the same size (10 sensors for example) is performed implicitly during the optimization process. The Simulated Annealing used in this study compares at each iteration two networks (of the same size) and retains the 'best one'. The networks are generated randomly like in Kovalets et al (2011) and Efthimiou et al (2017). Since the search space is quite large, the number of the compared networks is equivalent to the number of iterations. The comparison is based on a cost function named Normalized Errors Js and inspired from the renormalized data assimilation method. This cost function quantifies the quadratic distance between the observed and the simulated measurements according to the normalized Gram matrix H_w. The 'optimal network' produce the 'best' description of the observations (i.e. corresponds to the minimal quadratic distance) and permits a posteriori to reconstruct its origin. In figures 1, 2 & 3 is presented the evolution of the cost functions (trials 5, 11 & 19) during the optimization process. For these trials, ~ 3×10^4 networks of 10 sensors are compared. The challenge in our study is to design the networks without using a priori the parameters of the real source and without considering an acceptance level of networks quality (the solution is 'good' if it satisfies three fixed criteria of values $rH \leq 15$ m, $rV \leq 2.5$ m, $\delta q \leq 4$) as performed in Kovalets et al (2011) and Efthimiou et al (2017). These points are more clearly discussed in the revised text.*

Comment 2: Why we compare results of source inversion (distance to the true source, etc.) with 'optimal network' of 10 sensors with the results obtained by the full network (40 sensors)?

Reply: *The results obtained by the optimal networks of 10 and 13 sensors are compared as a posteriori with the original network of 40 sensors used in MUST experiment and evaluated for source reconstruction by using the renormalization technique (Kumar et al, 2015b). As in practice, the number of measurements is limited, this comparison allowed concluding that in urban areas, the reduction of networks size is possible and does not degrade significantly its efficiency in source estimation. For more details, the choice of the size of the network (10 and 13) is fixed after observing that an acceptable estimation of the source in majorities of the trials was enabled by using minimum 8 sensors. Also by using more than 13 sensors optimal networks, the errors in source parameters estimation are stable and does not improve significantly (Kouichi, 2017). For this reason, the optimized networks were constructed and evaluated for sizes 10 and 13 (1/4th and ∼ 1/3rd of the original network of 40 sensors) with the original large network. These points are more clearly discussed in the revised text.*

References

1) I.V. Kovalets, S. Andronopoulos, A.G. Venetsanos, J.G. Bartzis, Identification of strength and location of stationary point source of atmospheric pollutant in urban conditions using computational fluid dynamics model, Math Comput Simulat, 82 (2011) 244-257.

2) G.C. Efthimiou, I.V. Kovalets, A. Venetsanos, S. Andronopoulos, C.D. Argyropoulos, K. Kakosimos, An optimized inverse modelling method for determining the location and strength of a point source releasing airborne material in urban environment, Atmos. Environ., 170 (2017) 118-129

3) Kouichi, H. (2017), Sensors networks optimization for the characterization of atmospheric releases source, Theses, Université Paris Saclay, France.

4) Kumar, P., Feiz, A.-A., Singh, S. K., Ngae, P., and Turbelin, G.: Reconstruction of an atmospheric tracer source in an urban-like environment, 15 Journal of Geophysical Research: Atmospheres, 120, 12 589–12 604, https://doi.org/10.1002/2015JD024110, http://dx.doi.org/10.1002/ 2015JD024110, 2015b.

Response to the Reviewer #2

In this paper, the authors formulate a simulated annealing algorithm with a renormalization inversion algorithm coupled to a CDF flow and dispersion model and apply it to the Mock Urban Setting Test (MUST) tracer field experiment (which simulates an 'urban-like' environment). The aim of the work is to demonstrate how the inversion technique presented can be useful in optimally placing a smaller number of concentration samplers for quantifying a continuous point source with almost the same level of source detection ability as the original larger number of samplers. The paper is well written, but in my opinion requires a major revision. My comments are as follows:

The authors are grateful to the reviewer's remarks and thanking him/her for reviewing the manuscript. In light of the reviewer's all suggestions, the manuscript is revised. Reviewer's questions and remarks are repeated below (in red color) and our responses (in italic) follow each question.

Main comments

1) The MUST experiments took place under neutral to stable and strongly stable conditions. However, the CFD model used is for neutral conditions and does not include the effects of atmospheric stability over the urban area (the only stability effects included are through the specification of inflow boundary conditions). Atmospheric stability has a profound impact on dispersion and would thus influence the adjoint functions. The authors should discuss the consequences of its neglect on the results and the errors it introduces.

Reply: *We agree with the reviewer's remark that the atmospheric stability effects in the CFD model fluidyn-PANACHE were included through the inflow boundary conditions. The used version of fluidyn-PANACHE was not capable of incorporating the atmospheric stratification through surface cooling or heating and whatever stability effects are included through the inflow boundary conditions. The fluidyn-PANACHE includes a Planetary Boundary Layer (PBL) model that serves as the interface between the meteorological observations and the boundary conditions required by the CFD solver. The PBL model is composed of two parts: (i) a micro-meteorological model that computes fundamental physical characteristics of the PBL from routine meteorological observations, and (ii) a boundary layer model for prescribing the vertical profiles of wind speed, temperature, and turbulence. However, as discussed in our previous study (Kumar et al., 2015a), even with the specification of the stability dependent inflow boundary conditions only, the predicting concentrations from the CFD model are in good agreement with the measured concentrations in the MUST experiment for all 20 trials in different atmospheric stability conditions. This may be due to that the scale and the urban geometry of the MUST field experiment are not large enough for the requirement to resolve the atmospheric stratification through surface cooling or heating. And the stability effects included through the inflow boundary conditions were enough to include the stability effects on the concentrations and adjoint functions at such a small scale* *urban-like environment of the MUST field experiment. However, at microscales also, small irregularities can break the repeated flow patterns found in a regular array of containers with identical shape (Qu et al, 2011). In addition, uncertainties associated with the thickness and the properties of the material of the container wall also affect flow pattern and the resulted concentrations and adjoint functions (Qu et al, 2011). Also, for a real urban environment at the larger scales, the atmospheric stability will have a profound impact on dispersion and would thus influence the adjoint functions. And the stability effects through the specification of inflow boundary conditions only, may not be appropriate for those environments. In these scenarios, the CFD model should be capable of incorporating the atmospheric stratification through surface cooling or heating in real urban environments.*

A brief discussion about these is now included in the revised manuscript.

2) I have reservations about the usefulness of the methodology presented in real-world urban environments. The title of the paper states 'urban monitoring network' but there are no real urban configurations used. The MUST experimental domain was only 200 m x 200 m (with buildings represented by a grid of containers) which cannot quite represent an urban area in terms of scale, meteorological variability, or non-uniform terrain or roughness/canopy structure. So in a way the present study does not explore any aspects that are specific to urban environments. The authors should discuss this, particularly how their methodology could be applied and its limitations in real-world urban cases. Following on, the title of the paper should say 'urban-like' or something similar instead of 'urban'.

Reply: *We agree with the referee's remarks that the Mock Urban Setting Test (MUST) tracer field experiment was performed in an urban-like environment and cannot quite represent an urban area in terms of scale, meteorological variability, or non-uniform terrain or roughness/canopy structure. However, the MUST field experiment has been widely utilized for the validation of the atmospheric dispersion models in an urban-like environment. Although, as mentioned by the reviewer also, there are several limitations to utilize this experiment; but, the methodology presented here is general in nature to apply to a real urban environment also. The methodology involves the utilization of the CFD model which generally can include the effects of the urban geometry, meteorological variability, or non-uniform terrain or roughness/canopy structure in a real urban environment. Therefore the title that will appear on the revised version changed accordingly "Optimization of an Urban-like Monitoring Network for Retrieving an Unknown Point Source Emission". Also, the limitations of the present methodology, for its application in real-world urban cases are discussed in the revised version.*

3) There were a total of 40 concentration samplers. In their optimisation, the authors arbitrarily fixed the number of samplers to 13 and 10 and then determined the optimum positions of these reduced number of samplers from the original 40 samplers. A better question to answer would have been "what is the minimum number of samplers required and what their positions are in order to quantify the source with a given degree of confidence or accuracy?"

Reply: *The numbers of the sensors were not fixed arbitrarily. The trends of location error (E_l) and the ratio of the estimated to true source intensity (E_q) with the number of sensors from 4 to 16 are performed and the results are presented in Kouichi (2017). As already mentioned in the manuscript, the number of sensors in the optimized networks were reduced to 1/3rd (13 sensors) and 1/4th (10 sensors) of the total number of sensors (40) originally deployed because for some cases a small number of sensors could not allow to correctly reconstruct the source and divergences of the calculations have been noted. As an example for Trial 14, reconstructing the source by using a small number on sensors is not appropriate since 4, 5, or 6 sensors are not enough (E_l> 100 m and log(E_q) > 10E+17). Also, after a certain number of sensors in the network, the source term estimation is not improved significantly (see Figure 1). Thus, selecting 10 (1/4th) and 13 (1/3rd) number of sensors in the optimal networks ensures an acceptable estimate of the source for all the trials. These points are more clearly discussed in the revised manuscript.*

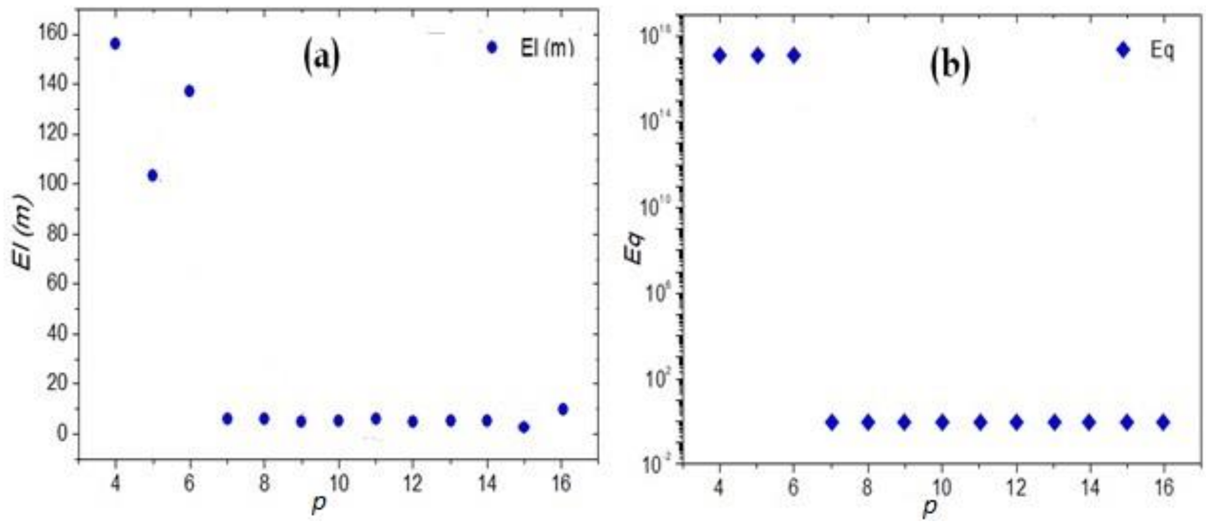

Figure 1: Errors in the estimation of the source (a) position and (b) intensity in Trial 14. Here p is the number of sensors

The present optimisation is based on fixed meteorological conditions in a trial. In a real situation, the network design would also depend on diurnal and spatial variability in meteorological conditions (e.g. wind direction) which may increase or decrease the optimum number of sites. This, however, is not in the scope of the present study. Perhaps as a future study, the authors may consider using data from full scale field measurements such as Salt Lake City Urban 2000 experiment.

Reply: *As the problem is complex, in this first study each meteorological situation is assumed as stationary and described by wind speed and direction and stability class. However, we agree with the referee, the network design would also depend on diurnal and spatial variability in meteorological conditions which may increase or decrease the optimum number of sites and also may change the 'best positions' to be instrumented by sensors. Indeed, we envisage as continuity of this work, to study the effect of the variability of the meteorological conditions. As suggested by the reviewer, we would like to utilize and validate the present* *methodology by using the data from full-scale field measurements such as Salt Lake City Urban 2000 experiment in a future study.*

4) Dense gas effects are included. How are they taken into account (or inverted) in the backward (i.e. retro plume) dispersion calculation for adjoint functions?

Reply: *Since the released tracer gas C_3H_6 in MUST field experiment is heavier than the air, a buoyancy model is used to model the body force term in the Navier-Stokes equations. The buoyancy model is suitable for the dispersion of heavy gases where density difference in the vertical direction drives the body force. Many attempts have been made in the literature to use CFD in simulating the dispersion of a negatively buoyant gas using a two-equation k-ε turbulence model (Sklavounos and Rigas, 2004; Tauseef et al., 2011, etc.). The fluidyn-PANACHE implementation of the k-ε model is derived from the standard high-Reynolds number (Re) form with corrections for buoyancy and compressibility (Launder, 2004; Hanjalic, 2005). The k-ε model computes the length and time scales from the local turbulence characteristics. Thus, it can model the turbulent flows subjected to both mechanical shear (obstacles, terrain undulations, canopy) as well as buoyancy (stability and buoyant/heavy gas plumes). For more information, the fluidyn-PANACHE is a three-dimensional (3-D) diagnostic model that solves Reynolds-averaged forms of the Navier-Stokes dynamics equations along with the equations describing conservation of tracer concentration, mass, and energy in the atmosphere (Fluidyn-PANACHE, 2010). As already mentioned in the manuscript, a detailed description of the fluidyn-PANACHE and its evaluation for the forward dispersion with the MUST field experiment was presented in our earlier paper (Kumar et al., 2015).*

5) What is the uncertainty in the source estimation results in Table 2? Is the approach capable of providing uncertainty estimates (like the Bayesian one)?

Reply: *With the present method, at this moment we cannot derive uncertainties like the Bayesian methods. However, we calculated posterior uncertainties on the source parameters estimation due to the measurements errors. In order to quantify the uncertainty, a 10% Gaussian noise was added at each measurement. Using the optimal networks 50 simulations for source characterization are performed for each trial. The average and the standard deviation of Eq and E_l are calculated and the results are present in Table 1 below. For the optimal networks, there is not an obvious trend and the uncertainties are in the same order of magnitude compared to the original network (40 sensors). The Table 2 of the actual version of the manuscript will be replaced by the following table 1 accordingly.*

Run No.	E_l^{40} (m)	E_l^{13} (m)	E_l^{10} (m)	E_q^{40}	E_q^{13}	E_q^{10}	Skeleton Sensors
1	*3.3 ±1.3*	*19.6 ±12.13*	*33.76 ±5.30*	*0.92 ±0.08*	*1.04 ±0.23*	*1.24 ±0.22*	*3*
2	*42.9 ±23.8*	*31.91 ±8.80*	*56.88 ±9.51*	*4.01 ±1.57*	*3.21 ±0.41*	*5.12 ±3.63*	*4*
3	*10.8 ±1.6*	*9.01 ±2.47*	*9.01 ±3.02*	*1.17 ±0.27*	*0.71 ±0.16*	*0.71 ±0.16*	*7*
4	*22.8 ±7.7*	*18.07 ±1.84*	*18.07 ±2.61*	*0.27 ±0.35*	*0.83 ±0.21*	*0.83 ±0.26*	*6*
5	*21.9 ±2.1*	*2.13 ±2.54*	*11.56 ±4.21*	*0.57 ±0.07*	*0.95 ±0.05*	*0.67 ±0.05*	*6*
6	*5.0 ±1.6*	*6.96 ±0.19*	*6.96 ±0.00*	*2.14 ±0.60*	*1.04 ±0.06*	*1.04 ±0.04*	*7*
7	*12.4 ±9.1*	*18.85 ±9.08*	*12.99 ±1.67*	*0.41 ±0.49*	*3.11 ±0.51*	*1.06 ±0.07*	*4*
8	*15.8 ±12.1*	*12.86 ±1.28*	*15.79 ±1.05*	*2.22 ±0.90*	*1.32 ±0.34*	*1.76 ±0.11*	*6*
9	*7.7 ±1.2*	*8.20 ±0.35*	*8.08 ±0.00*	*1.37 ±0.07*	*3.06 ±0.17*	*7.55 ±0.39*	*5*
10	*8.8 ±3.0*	*8.00 ±4.57*	*8.00 ±5.68*	*1.08 ±0.19*	*1.08 ±0.77*	*1.08 ±1.07*	*8*
11	*19.8 ±5.0*	*17.19 ±12.00*	*17.19 ±7.06*	*1.67 ±0.12*	*1.62 ±0.40*	*1.62 ±0.26*	*3*
12	*7.4 ±6.6*	*5.43 ±11.69*	*10.22 ±9.10*	*0.95 ±0.06*	*0.85 ±0.28*	*0.2 ±0.04*	*4*
13	*7.7 ±0.6*	*8.63 ±4.36*	*8.63 ±3.86*	*0.97 ±0.07*	*0.78 ±0.18*	*0.78 ± 2.05*	*4*
14	*2.2 ±1.9*	*5.50 ±2.98*	*5.50 ±3.88*	*1.42 ±0.17*	*0.88 ±0.24*	*0.88 ±0.40*	*7*
15	*1.1 ±1.0*	*30.23 ±2.14*	*37.98 ±0.72*	*1.88 ±0.09*	*0.57 ±0.07*	*0.17 ±0.01*	*7*
16	*26.7 ±4.9*	*63.04 ±6.84*	*29.80 ±9.86*	*1.70 ±0.06*	*0.29 ±0.06*	*0.67 ±0.23*	*5*
17	*7.0 ±1.9*	*14.07 ±2.78*	*23.05 ±10.44*	*0.90 ±0.05*	*1.10 ±0.04*	*1.52 ±0.16*	*6*
18	*14.3 ±11.0*	*12.83 ±4.18*	*12.83 ±4.61*	*1.15 ±0.46*	*1.15 ±0.16*	*1.15 ±0.21*	*6*
19	*22.3 ±6.4*	*10.77 ±4.25*	*13.46 ±4.8*	*1.76 ±0.16*	*0.99 ±0.20*	*0.83 ±0.25*	*6*
20	*32.5 ±1.8*	*45.23 ±1.78*	*44.29 ±0.31*	*0.83 ±0.04*	*1.68 ±0.06*	*1.56 ±0.06*	*7*

Table1. Source estimation results from the different monitoring networks for each selected trial of the MUST field experiment

6) How does the uncertainty in the results in Table 2 change as the number of samplers is changed? Have you included model and measurement uncertainties in the methodology?

Reply: *A general relationship between the number of samplers and the uncertainties is not obvious. We noticed that changing size of the network (increasing or decreasing the number of sensors) can lead to the growth or diminution of the uncertainties in the source parameters estimation. As an example in Table 1, for Trial#7 uncertainties grow while for Trial#17 uncertainties diminish.*

Accordingly to the answers of questions 5 and 6, results and interpretations of the effect of measurements errors on the source parameters estimation are included in the revised text.

7) Section 2.3: Is there a sensitivity of the source estimation / optimisation to how the weight function is selected? Could there be any other choices of the weight function?

Reply: *The weight function is selected to minimize the information retrieved from the observations thus avoiding inversion artifacts close to the detectors positions. This optimal renormalizing function denoted $\phi(x)$ is unique as demonstrated by Issartel (2004). However, the sensitivity of the source estimation is essentially due to the information provided by each vector of measurements.*

8) Did you specify any a priori bounds on the estimated source position and source emission rate? If yes, what were they?

Reply: *In this study, we do not require to specify any a priori bounds on the estimated source position and source emission rate in the renormalization inversion technique.*

9) What is the advantage of the present technique compared to, say, the Bayesian approach which also provides probability associated with the solution?

Reply: *The technique used in this study does not require a priori information about the source (i.e. location and intensity) or about the measurements (i.e. knowledge of the observation-Error Covariance Matrices). The renormalization is a deterministic inversion method compatible with upstream offline preparation for network implementation and compatible with rapid implementation for the monitoring operation phase for local-scale applications around sensitive sites. Also, this method can be used to estimate a point or distributed source which can expand the cases studied.*

10) Page 3, line 15: 'The Gaussian models are unable to capture. . .' While this may be generally true, a well formulated Gaussian plume model can describe idealised urban dispersion (e.g. Huq and Franzese, BLM, 147, 102-121, 2013).

Reply: *Corrected accordingly as 'In general, the Gaussian models are unable to capture. . .'*

11) Section 5: Was the CFD model validated using the MUST data for its ability to simulate the measured concentrations?

Reply: *As already mentioned in the manuscript, the ability of the CFD model to simulate the measured concentrations using the MUST data and the prediction errors of the forward simulations used in this study were discussed in our previous study (Kumar et al., 2015).*

12) Source position was calculated. Does it include the source height too? Was source height a free parameter or a fixed one?

Reply: *The source height was not calculated in this study. The computations were carried out in the 2-dimensional domain on a horizontal plane corresponds to an altitude of known source height Hs. Accordingly, the vertical dimension was eliminated in the formulations and the computations. Consequently, the adjoint functions were chosen as steady state retroplumes on the horizontal cross-section area passing through a plane z = Hs. The assumption with respect to the vertical structure of the problem is useful to estimate the ground level sources or the emission sources along a horizontal cross-section area passing through a fixed vertical level. However, in this study, the problem of vertical structure (i.e. the height of a source) in three-dimensional space of an urban area is not addressed. In reality, an altitude of a release (i.e. source height) is also not known and required to estimate along with the projected release location on the ground surface and the release rate (Kumar et al., 2016). We envisage to include the height of the source in a future study.*

Other comments

13) Page 2, line 14: What is 'an NP-hard problem'?

Reply: *The problem of sensors network optimisationis NP-Hard (i.e. Non-deterministic Polynomial-time hardness) as shown by (Ko et al., 1995), which means that it is difficult for an exhaustive search algorithm to solve all instances of the problem because it's need a considerable time.*

14) Page 2, line 35: 'probabilities' should be 'probability'.

Reply: *Corrected. We have now carefully checked the manuscript to eliminate possible linguistic errors.*

15) Page 3, line 8: ‘required’ should be ‘require’.

Reply: *Corrected.*

16) Page 3, line 10: ‘the continuous’ should be ‘continuous’.

Reply: *Corrected*.

17) Page 3, line 23: ‘was’ should be ‘is’.

Reply: *Corrected.*

18) Is the optimisation methodology presented only valid for a single source?

Reply: *In this study, the presented optimization methodology is only valid for a single source. Nevertheless, it is possible to consider the optimization for multiple sources. We envisage that evaluation in the future.*

19) Page 7, line 3: The term temperature should be put in quotes as this is not a real temperature in the present context.

Reply: *Changed accordingly.*

20) Page 9, line 2: ‘stopped’ should be ‘is stopped’.

Reply: *Corrected.*

21) Figures 1 and 3: Why some of the 40 samplers locations do not coincide in these figures?

Reply: *In the schematization of the MUST experiment, the position of the tenth detector of the fourth row was slightly shifted from its true position. Figure 1 in actual manuscript version is adjusted accordingly as shown in figure 2 below.*

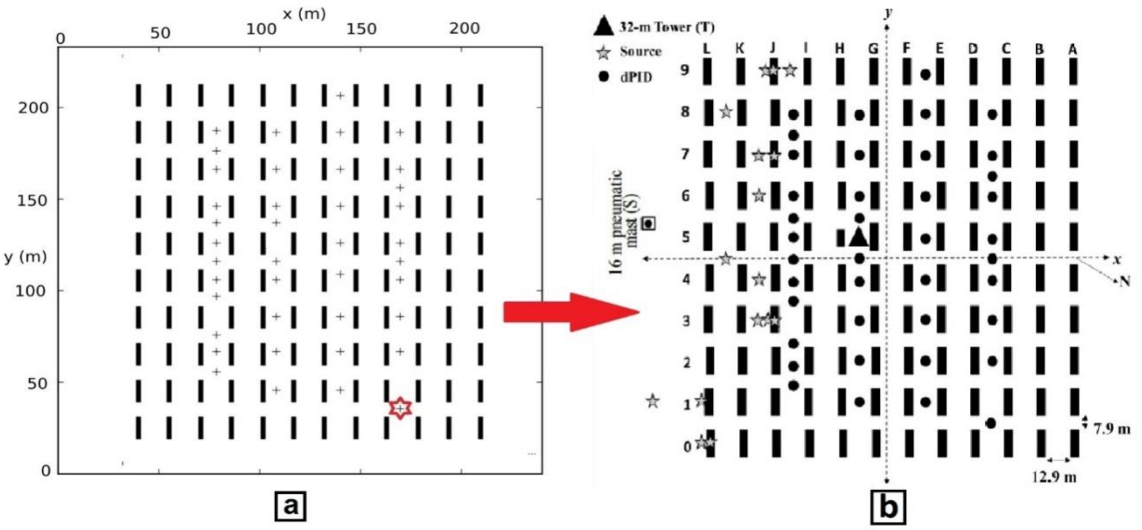

Figure 2: Schematization of the MUST experiment: (a) correct version (b) adjusted version

22) Is the code for simulated annealing algorithm with the renormalization inversion technique available?

Reply: Yes *the codes are available for one trial as an example.*

References

Fluidyn-PANACHE, 2010. User Manual. FLUIDYN France / TRANSOFT International, version 4.0.7 Edition.

Hanjalic, K., 2005. Turbulence and transport phenomena: Modelling and simulation. In: Turbulence Modeling and Simulation (TMS) Workshop. Technische Universitat Darmstadt.

Issartel, J.-P. Emergence of a tracer source from air concentration measurements, a new strategy for linear assimilation. Atmospheric Chem. Phys. 5, 249–273 (2005). URL http://www.*atmos-chem-phys.net/5/249/2005/. DOI 10.5194/acp-5-249-2005.*

Ko, C.-W., Lee, J., Queyranne, M., 1995 An exact algorithm for maximum entropy sampling. Operational Research, 43, 684–691. URL https://doi.org/10.1287/opre.43.4.684.

Kouichi, H. (2017). Sensors networks optimization for the characterization of atmospheric releases source, Theses, Université Paris Saclay, France. https://hal.archivesouvertes.fr/tel-01593834v2

Kumar, P., Feiz, A.-A., Ngae, P., Singh, S. K., Issartel, J.-P., 2015. CFD simulation of short-range plume dispersion from a point release in an urban like environment. Atmospheric Environment 122, 645 – 656. URL http://www.sciencedirect.com/science/article/pii/S1352231015304465

Kumar, P., Singh, S. K., Feiz, A.-A., Ngae, P., 2016. An urban scale inverse modelling for retrieving unknown elevated emissions with building-resolving simulations. Atmospheric environment, 140, 135-146. URL https://doi.org/10.1016/j.atmosenv.2016.05.050

Launder, B., 2004. Turbulence modelling of buoyancy-affected flows. In: Singapore Turbulence Colloquium.

Qu, Y., Milliez, M., Musson-Genon, L., &Carissimo, B. (2011). Micrometeorological modeling of radiative and convective effects with a building-resolving code. Journal of applied meteorology and climatology, 50(8), 1713-1724.

Sklavounos, S., Rigas, F., 2004. Validation of turbulence models in heavy gas dispersion over obstacles. Journal of Hazardous Materials 108 (1), 9 – 20. URL http://www.sciencedirect.com/science/article/pii/S0304389404000494

Tauseef, S., Rashtchian, D., Abbasi, S., 2011. CFD-based simulation of dense gas dispersion in presence of obstacles. Journal of Loss Prevention in the Process Industries 24 (4), 371 – 376. URL http://www.sciencedirect.com/science/article/pii/S0950423011000222

Response to the Reviewer #3

The subject of this paper is challenging and very timely; certainly, we would like to know how to monitor the spread of pollutants in the urban milieu as efficiently and accurately as possible. In order to accomplish this task, the Authors derive a method based on the combination of optimization techniques, inverse tracers transport modelling and Computational Fluid Dynamics. The subject is very difficult and there are very few papers addressing the problem in a comprehensive manner; for this reason it is justified to consider publication of this study.

We would like to thank Dr. Pudykiewicz for his careful consideration of this manuscript and for his helpful and insightful comments. We have carefully considered his comments and worked to include them in the revised version of the manuscript according to the proposed suggestions.

Please find below the responses to his comments.

1) ‘The Authors attempt to analyze two canonical problems: - Identification of the unknown source - Optimization of the measuring network. These two problems are mutually exclusive. Furthermore, they have different cost functionals defined on different vector spaces and, consequently, the set of control parameters is not the same for each case. This important distinction is overlooked in the paper and it is advisable to modify the text by precisely defining the functionals and the control variables.’

Reply: *In this study two canonical problems are considered:*

a) Identification of the unknown source: the source term estimation STE is studied in the framework of a parametric approach using the renormalization technique. Here the challenge is to determine the parameters of the source (intensity and position) using any measurements vector (in practice the number of measurements is limited). Based on retroplumes (using sensors locations and CFD model in backward mode), we first determine the optimal renormalized Gram matrix $\boldsymbol{H}_w$*, for which an optimal weight function is required. This optimal weight function that verifies the renormalization condition minimize the information retrieved from the observations thus avoiding inversion artifacts close to the detectors positions. As the renormalization is a data assimilation method, the cost function to minimize is defined as the quadratic distance between the observed and the simulated measurements according to the* $\boldsymbol{H}_w$ *norm.*

b) Optimization of the measuring network: here, the optimization consists of selecting the best positions to be instrumented by the sensors among potential locations. This choice is operated in a space of search constituted of all possible networks (of a specific size) and based on a cost function that describes quantitatively the quality of the networks. The optimal network has the lowest quadratic distance between the observed and the simulated measurements according to the $\boldsymbol{H}_w$ *norm. This optimal (or near-optimal) network is obtained using the*

Simulated Annealing (SA) algorithm. The data here are the measurements and the according sensors locations.

These canonical problems are coupled at each iteration during the searching process.

The text of the revised manuscript is accordingly modified to clarify this important point.

2) 'The problem of optimization of the network is solved using the simulated annealing algorithm. The technique has been introduced to the computational physics over sixty years ago in the classic paper: Metropolis, N.; Rosenbluth, A. W.; Rosenbluth, M.; Teller, A. H.; and Teller, E. "Equation of State Calculations by Fast Computing Machines." J. Chem. Phys. 21, 1087-1092, 1953. Despite that the original formulation is rooted in the basic principles of physics, the reviewed paper, concerned with the network optimization, is missing the physical interpretation of the Simulated Annealing. The description of the technique can read as follows: The algorithm of simulated annealing is initiated by starting from an admissible network. At the subsequent steps, the system moves to another feasible network, according to a prescribed probability, or it remains in the current state. It is crucial to explain how this probability is calculated. The mobility of the random walk depends on a global parameter T which is interpreted as temperature. The initial values of T are large, allowing free exploration of large extents of the state space (this corresponds to the "melted state" in terms of the kinetic theory of matter). In the subsequent steps, the temperature is lowered allowing the algorithm to reach a local minimum.'

Reply: *The SA algorithm is a random optimization technique based on an analogy with thermodynamics. For the SA, each network of p sensors is considered as a state of a virtual physical system, and the objective function is interpreted as the internal energy of this system in a given state. According to statistical thermodynamics, the probability of a physical system to being in a state β follows the Boltzmann distribution $P_\beta = \frac{1}{Z} exp(\frac{-\Delta E_\beta}{K_B T})$, where Z is the partition function, E_β is the internal energy, T is the temperature at the state β and K_B is the constant of Boltzmann. By analogy, the physical quantities (temperature, energy, etc.) become pseudo-quantities and during the minimization process, the probabilistic treatment consists to accept a new network selected in the neighborhood of the current network following the probability $P = exp(\frac{-\Delta J}{T})$, where ΔJ is the cost difference between the new and the current configurations. At high temperature, the SA performs a coarse search of the space of global states, avoids local minima and finds a good minimum. As the temperature is lowered, the search becomes fine in the neighborhood of the already determined minimum and the SA reaches a better minimum.*

As suggested, we have included this physical interpretation of the Simulated Annealing in the revised manuscript.

3) The main characteristic of SA is relatively fast convergence but, unfortunately, it is not possible to prove that the minimum of the cost functional is global. There are several others stochastic minimization methods which can be explored; it is possible that they are potentially more applicable in the context of the monitoring of air pollutants.

Reply: *It is clear that for all the metaheuristic algorithms (such as the SA), it is not possible to prove that the minimum of the cost functional is global. This question is crucial for us, for this reason, we plan in the future to study the degree of confidence on the 'optimal networks'. Nevertheless, before retaining the SA as an optimization technique, we tested and compared the results obtained by Genetic Algorithm (GA) and SA based on the normalized error cost function (Kouichi, 2017). These algorithms of different search technics (SA probabilistic & GA evolutionary) are evaluated for the reconstruction of a source in a wind tunnel (DYCE experiment (Lepley et al., 2011). The optimization consisted in selecting the best positions for sensors implantation among 27 potential positions scattered in the Wind Tunnel. The results show that the optimal networks retained by the GA and the SA are quantitatively (figure 1) and qualitatively (figure 2) comparable. The errors in source parameters estimation by using the optimal networks of 3 to 13 sensors are presented in figure 1 below. The SA has advantageous because it is relatively easy to implement and takes smaller computational time in comparison to GA. Both SA and GA optimization algorithms in the framework of our approach (based in the renormalization theory) has little influence on the estimation of the parameters of a source.*

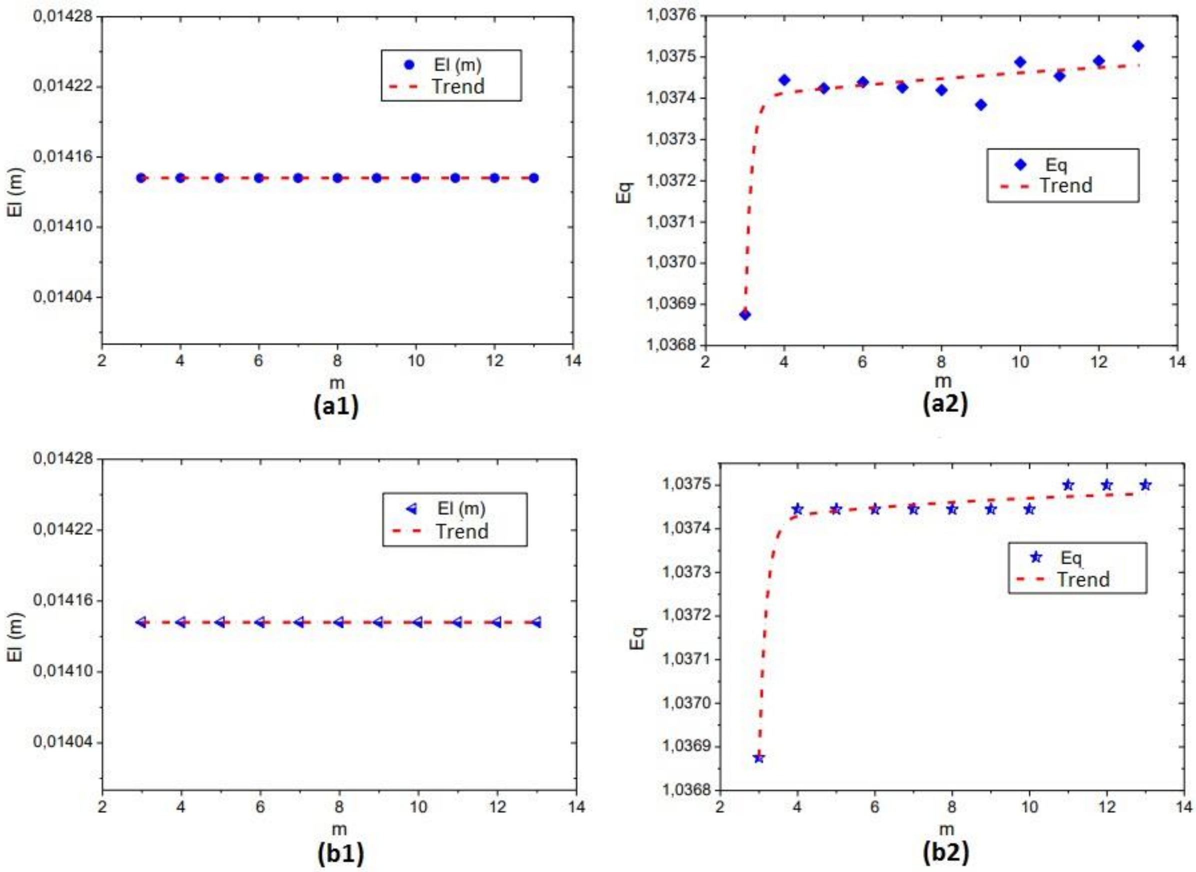

Figure 1: Error of source parameters estimation for (a) SA (b) GA in the DYCE wind tunnel experiment. Here m is the number of sensors, E_l and E_q respectively denote the location error (m) and the ratio of the estimated to true source intensity

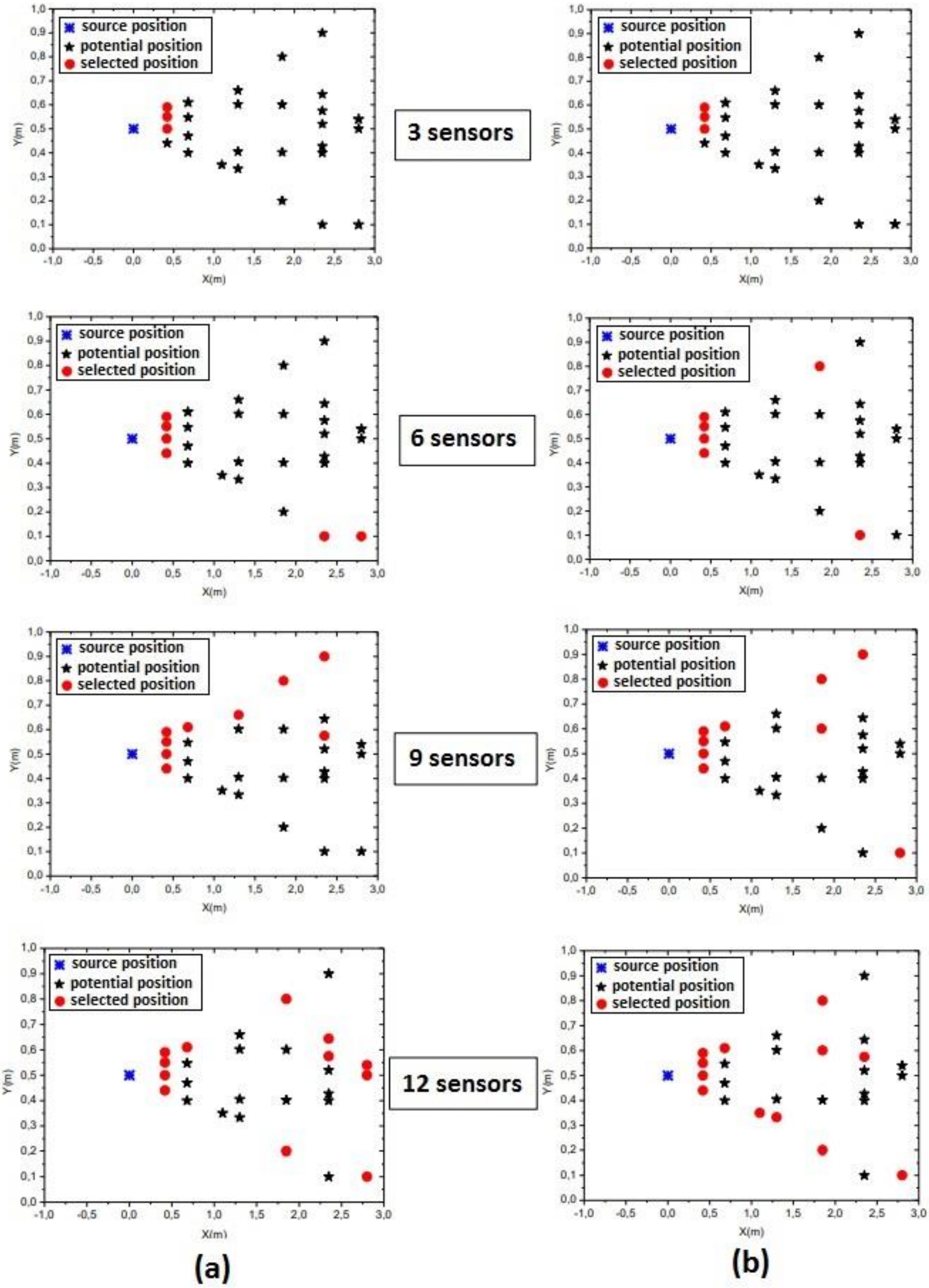

Figure 2: Optimal networks (m = 3, 6, 9 and 12) obtained by (a) Simulated Annealing SA and (b) Genetic Algorithm GA

4) The problem of selection of the initial admissible network and the role of stratification should be discussed. It is well known that the flow around and above complicated structures is characterized by a complex topology. After some analysis of the literature, I'm convinced that the solution of the network optimization depends strongly on the flow Froude number. The relevant information on the flow in the vicinity of a structure is discussed in the literature, please see for example https://link.springer.com/article/10.1007/s10652-016- 9470-3. It would be interesting to present some figures describing both wind and potential temperature fields from the CFD model used in the study.

Reply: *The initial admissible network is selected following the trends of location error (E_l) and ratio of the estimated to true source intensity (E_q) with the number of sensors from 4 to 16 are performed and the results are presented in Kouichi (2017). As already mentioned in the manuscript, the number of sensors in the optimized networks were reduced to 1/3rd (13 sensors) and 1/4th (10 sensors) of the total number of sensors (40) originally deployed because for some cases a small number of sensors could not allow to correctly reconstruct the source and divergences of the calculations have been noted. As an example for Trial 14, reconstructing the source by using a small number on sensors is not appropriate since 4, 5, or 6 sensors are not enough (E_l> 100 m and log(E_q) > 10E+17). Also, after a certain number of sensors in the network, the source term estimation is not improved significantly (see Figure 3). Thus, selecting 10 (1/4th) and 13 (1/3rd) number of sensors in the optimal networks ensures an acceptable estimate of the source for all the trials. These points are more clearly discussed in the revised manuscript.*

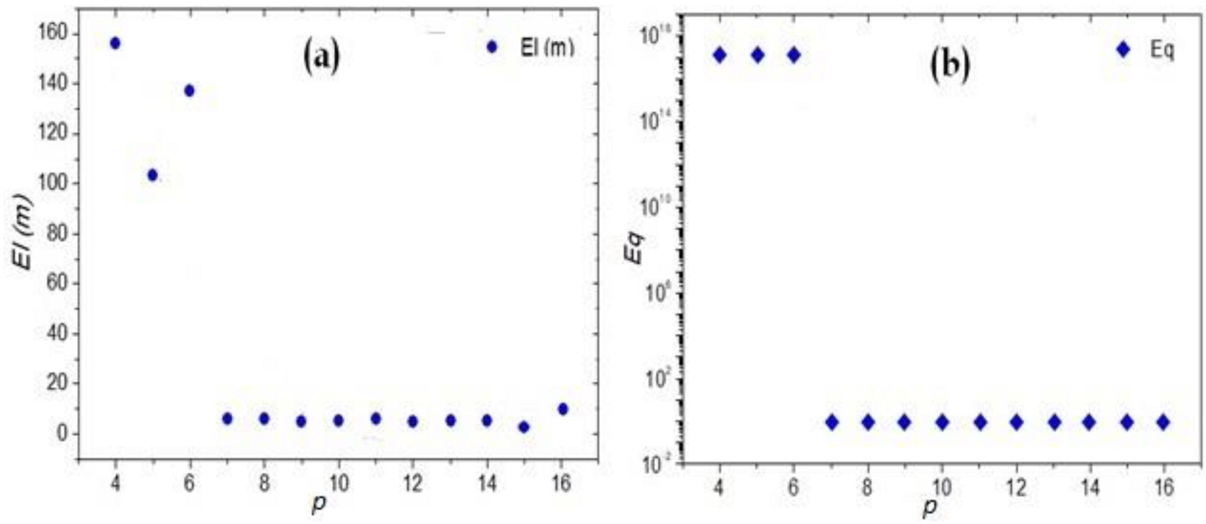

Figure 3: Errors in the estimation of the source (a) position and (b) intensity in Trial 14. Here p is the number of sensors

The atmospheric stability effects in the CFD model fluidyn-PANACHE were included through the inflow boundary conditions. We had already analyzed the importance of the proper inflow boundary conditions for wind and turbulence variables on forward and backward atmospheric dispersion in an urban area (Kumar et al., 2015). Accordingly, Gryning et al. (2007) wind profile and an approximate analytical solution of the one-dimensional k-ε prognostic equation (Yang et al., 2009) for the turbulence profiles were used for inflow *boundary. Gryning et al. (2007) wind profile is composed of the three different length scales in the surface, middle, and upper layers of the atmospheric boundary layer (ABL), and is applicable in the entire ABL. It was also noted that Gryning's wind profile is not applicable in the trials (number 4, 5, and 6 of the MUST field experiment) of very stable atmospheric conditions. Thus, a wind profile based on the similarity function proposed by Beljaars and Holtslag (1991) was used in these trials. The Monin-Obukhov similarity theory-based logarithmic temperature profile was used to describe its vertical variation in neutral and stable conditions in the MUST field experiment. Since the coefficients in approximated analytical profiles of k and ε are estimated by fitting the observed values of k, the turbulence profiles follow the actual representation of k in each trial of the MUST experiment (Kumar et al., 2015).*

More generally, in pollutant dispersion problems, when a proper level of turbulence intensity is important at the upwind side of the obstacles, the commonly used techniques are based on setting up simplified forms of inlet TKE (Santos et al., 2009), dynamical recycling (Tomas et al., 2015) or smooth inflow with generic downwind roughness elements (Tomas et al., 2016). Such conditions mostly affect the intensity of vertical mixing and the rate of boundary layer growth, decisive factors in determining concentrations of pollutants emitted within the urban canopy (Korycki et al., 2016). We think that these effects are beyond the scope of this work and could be further explored for the future. These discussions are now included in the revised manuscript,

We also present in the revised manuscript figures describing wind fields from the CFD model for the trials 4, 11 and 19. As an example, in figure 4 below is showed the wind velocity vectors around some containers for the trial 11.

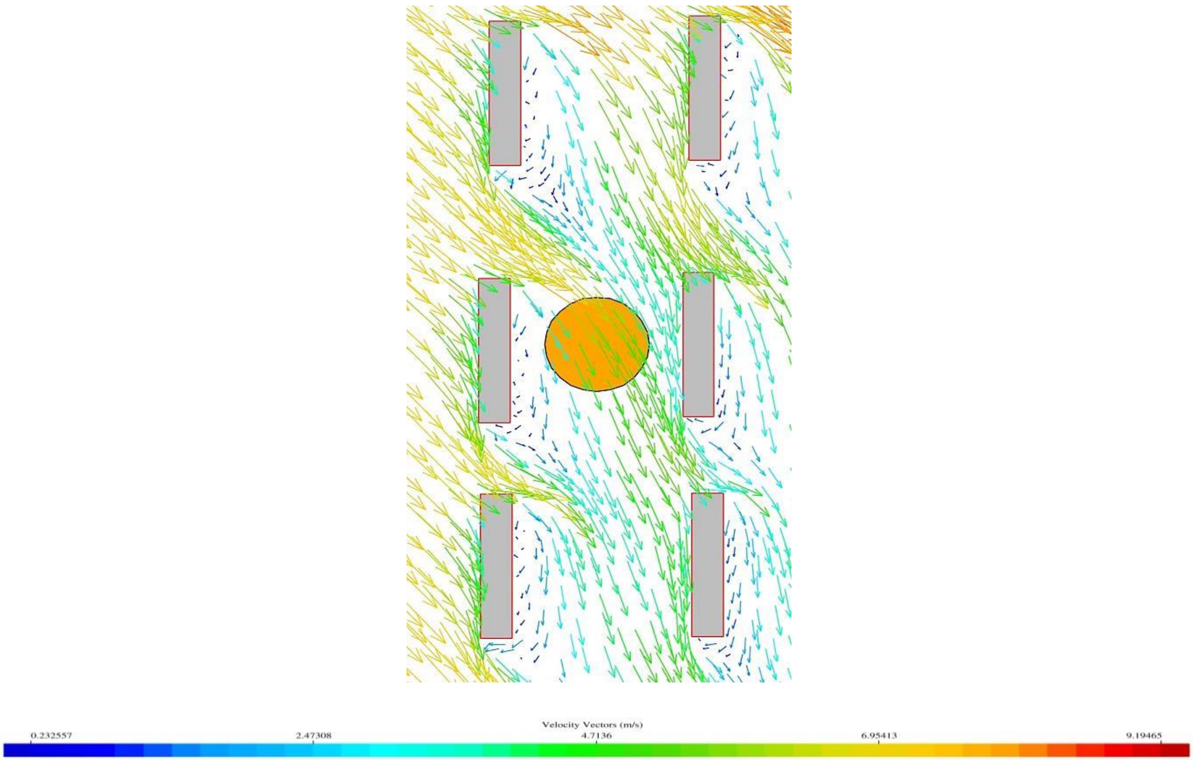

Figure 4: Wind velocity vectors for the trial 11

References

Beljaars, A., Holtslag, A., 1991. Flux parameterization over land surfaces for atmospheric models. J. Appl. Meteorol., 30 (3), 327-341, http://dx.doi.org/10.1175/1520-0450(1991)030<0327:FPOLSF>2.0.CO;2

Gryning, S.-E., Batchvarova, E., Brmmer Jr., B., Gensen, H., Larsen, S., 2007. On theextension of the wind profile over homogeneous terrain beyond the surfaceboundary layer. Bound. Layer Meteorol. 124 (2), 251-268. http://dx.doi.org/10.1007/s10546-007-9166-9

Korycki, M., Łobocki, L., Wyszogrodzki, A., 2016. Numerical simulation of stratified flow around a tall building of a complex shape Environ Fluid Mech, 16, 1143–1171, DOI 10.1007/s10652-016-9470-3

Kouichi, H., Jul. 2017. Sensors networks optimization for the characterization of atmospheric releases source. Thesis, Université Paris Saclay, France. URL https://hal.archives-ouvertes.fr/tel-01593834

Kumar, P., Feiz, A.-A., Ngae, P., Singh, S. K., Issartel, J.-P., 2015. CFD simulation of short-range plume dispersion from a point release in an urban like environment. Atmospheric Environment 122, 645 – 656.
URL http://www.sciencedirect.com/science/article/pii/S1352231015304465

Lepley, J. J., Lloyd, D., Robins, A., Wilks, A., Rudd, A., Belcher, S., (2011). Dynamic sensor deployment for the monitoring of chemical releases in urban environments (DYCE), Proc. of SPIE, 8018(12), 1-11, doi:10.1117/12.883373.

Santos, J.M., Reis, N.C., Goulart, E.V., Mavroidis, I., 2009. Numerical simulation of flow and dispersionaround an isolated cubical building: the effect of the atmospheric stratification. Atmos Environ43:5484–5492. doi:10.1016/j.atmosenv.2009.07.020

Tomas, J.M., Pourquie, M.J.B.M., Jonker, H.J.J., 2015. The influence of an obstacle on flow and pollutantdispersion in neutral and stable boundary layers. Atmos Environ 113:236–246, https://doi.org/10.1016/j.atmosenv.2015.05.016

Tomas, J.M., Pourquie, M.J.B.M., Jonker, H.J.J., 2016. Stable stratification effects on flow and pollutant dispersion in boundary layers entering a generic urban environment. Bound Layer Meteorol 159(2):221–239, https://doi.org/10.1007/s10546-015-0124-7

Yang, Y., Gu, M., Chen, S., Jin, X., 2009. New inflow boundary conditions formodelling the neutral equilibrium atmospheric boundary layer in computationalwind engineering. J. Wind Eng. Industrial Aerodyn. 97 (2), 88-95.
http://www.sciencedirect.com/science/article/pii/S0167610508001815.

Response to the Short Comment #SC4

We thank to our former colleague Dr. Sarvesh Singh in the LMEE Laboratory with whom we have also published many research papers as a coauthor, for his detailed reading of our paper. We are grateful to him, despite the fact he is perhaps a bit too personally involved, reading and commenting so abundantly our work, pointing out the weakness of some difficult explanations given too quickly. He has a good practice in inverse modeling for the air pollutant source reconstruction in flat and homogeneous terrains. However, we understand that this multidisciplinary study which requires wide knowledge, not only of the inverse problem but also of the CFD modelling, optimization, and experience in engineering, can lead to some confusion and misunderstanding. Below we tried to answer (in italic form) to all of his comments (in red color), also many of his comments were repeated several times asking the similar question again and again.

Comment: The manuscript highlights an interesting and challenging problem related to the optimization of sensor networks in the context of a point source reconstruction. In general, the optimization of monitoring network consists of two important issues: (i) reducing the number of receptors and (ii) finding an optimal design of the arrangement of the monitoring network. Here, the study deals only with selecting a reduced set of number of receptors among an already established monitoring network, which is very limited form of a real problem.

Reply: *The optimization of monitoring network doesn't consist in general two important issues: reducing the number of receptors and finding an optimal design of the arrangement of the monitoring network, this affirmation is very simplistic. Fundamentally, the optimization of monitoring networks problems may concern:*

*1. <u>First deployment:</u> This case is the more complex and consists in defining different interesting areas (monitored area, vulnerable area, danger area, the potential locations, etc.) before optimizing the network. This problem cannot be dealt with in general, because the studied zones change according to the situation (industrial zone, target of an aggression from the external, etc.). Once the search space is defined (i.e. the candidate locations for the sensors implantation), the problem can concern finding the best configuration of a minimal number of sensors (similar to problem 3 below) or the best spatial arrangement of a predetermined number of detectors (in some cases, for example, the protection against eventual terrorist attack, **a limited number of sensors is not important** and the security must be guaranteed by the maximum means).*

2. <u>Updating an existing network:</u> This problem consists in changing the sensors positions in the interesting area for the specific needs (such as an important variation of the meteorological situations after a long time the network is designed) without changing the size of the networks (i.e. the number of sensors).

3. <u>Reducing the size of an existing network:</u> The challenge here is to determine the optimal size of the network and the best locations for the sensors implantation. Here the original network is considered as the search space.

4. <u>Increasing the size of an existing network:</u> This problem consists in determining the best positions to add to a set of sensors already placed on a site. The number of detectors to add can be prefixed or included in the optimization problem (i.e. must be determined).

The detailed problems are independent and each one of them have its own requirements.

It is also important to know that the optimization of sensors networks depends on the network type:

a. Mobile network deployed only on emergency: Here the detectors are rapidly deployed specifically for collecting the information (i.e. measurements) to be used for a specific need (neutralize the source, refurbishment an installation on industrial site, etc.). In this case, the meteorological conditions (as wind speed and direction, etc.) can be known in real time from the available observations or from numerical weather forecasting models and can be assumed as stationary. The optimization, in this case, can be performed in real time if the interesting area is not complex and the calculation can be conducted quickly in a very short time (using Gaussian model and an optimization algorithm for example). If the domain is complex (i.e. contains several obstacles), CFD model must be used to include the effect of the obstacles, the optimal locations to be instrumented by the sensors must be determined in upstream off-line.

b. Permanent mobile network: Here the vulnerable area is monitored permanently by detectors embarked in mobile systems (such as drones or robots). The optimization, in this case, consists in determining the best locations following the situation (meteorological conditions, the presence of a danger, detection of an accident, etc.).

c. Permanent static network: Here the vulnerable area is monitored permanently by a fixed network that must be efficient regardless of the meteorological situations. The optimal design consists in finding the best arrangement of the detectors (the number can be minimal or prefixed).

As a conclusion, the optimization of monitoring network in an urban environment is a complex problem that must be deal with the proper use of the inverse modeling, CFD modeling, and optimization techniques. The present study deals with the above cases (3) and (a). As also pointed out by Dr. Pudykiewicz, one of the reviewers of this paper and a distinguished scientist in this field, the subject of this study is challenging, very timely, and very difficult and there are very few papers addressing the problem in a comprehensive manner. In order to accomplish this task, we derived a method based on the combination of optimization techniques, inverse tracers transport modeling, and Computational Fluid Dynamics. So the remark of Dr. Singh that the study is a very limited form of a real problem is not true.

For more detail we have cited below some studies that can help to understand the challenges and the methods that can be used in the context of our work:

- *(Chen et al 2012): Optimization of water quality monitoring network in a large river by combining measurements, a numerical model and matter-element analyses.*
- *(Ainslie et al 2009): Application of an entropy-based Bayesian optimization technique to the redesign of an existing monitoring network for single air pollutants.*
- *(Mofarrah & Husain, 2010): A holistic approach for optimal design of air quality monitoring network expansion in an urban area.*
- *(Lepley et al 2011): Dynamic sensor deployment for the monitoring of chemical releases in urban environment.*

- *(Le et al, 2003): Designing networks for monitoring multivariate environmental fields using data with monotone pattern.*
- *(Jiang et al, 2007): Optimization of mobile radioactivity monitoring networks.*

Comment: The authors have already published the inversion methodology and simulated annealing algorithm (SA) with its application to wind tunnel experiment in Kuichi et al. (2016). The present study shows a similar application in an urban terrain field experiment by using a CFD model.

Reply: *'' Kuichi et al. (2016)'', do you mean Kouichi et al. (2016)?*

This comment of Dr. Singh is not completely true and also misleading as in the study of Kouichi et al. (2016), which is, in fact, a conference paper, the dispersion experiment of the gas and the modeling study were performed in very idealized conditions in a wind tunnel (standard deviation adjusted specifically for the wind tunnel, wind speed fixed according to the best results, measurements far from the boundary layer, dispersion in a homogeneous space without obstacles, etc.). All these aspects simplify the complexity of the optimal design problem and don't lead to a fine analysis of the locations importance on the reconstruction of the source parameters. The current study of the networks optimization in view of the source reconstruction in the urban domain is a very complex and challenging problem and the renormalization inversion method has never been the subject of this study, this clearly justifies the originality of this work. With proper citations of our earlier works, in this study, we never claimed to present the inversion methodology. In fact, the earlier source reconstruction results were presented for comparison purposes only with proper citation of that work. In this study, we derived a methodology for designing the optimal monitoring networks ***in an urban-like environment*** *based on the combination of optimization techniques, inverse tracers transport modeling and Computational Fluid Dynamics. Dr. Singh comment that this is just an application in an urban terrain field experiment by using a CFD model, cannot be justified as Dr. Pudykiewicz also pointed out that this study is challenging and very difficult and there are very few papers addressing the problem in a comprehensive manner. In fact, the complexity of the problem increases manifold for urban environments where simple analytical or Gaussian models have limitations and cannot apply to such complex environments. This study presents a method for designing the optimal monitoring networks in an urban-like environment.*

Comment: It does not involve any new development in the model or inversion / optimization algorithm.

Reply: *Fundamentally an optimization study does not require development in the used methods or algorithms but it is ensured by three essential phases:*

1. Choice of an objective function: (also known as cost functions), in our case this function is the optimality criterion which describes the quality of a network and which is in agreement with the defined problem (mobile or static network, for reconstruction of a source or for other need, etc.).

2. The problem statement: this consists in defining how the optimization problem is approached (i.e. discrete or continuous search areas, definitions of spatial zones, etc.).

3. The choice of the optimization algorithm: which is generally in coherence with the phase 2 (Determinist optimization, Hard optimization, etc.)

The complexity of the optimization problems is in the well definition of these three phases especially the choice of the optimality criterion and also in the implementation and the exploitation of the retained techniques. In this study, we never claimed any development in the inversion or optimizations algorithms as these techniques were already available in the literature. We derived a methodology for designing the optimal monitoring networks in an urban-like environment which is based on the combination of optimization techniques, inverse tracers transport modeling, and Computational Fluid Dynamics. Which attests to a new development for optimally designing the sensors monitoring network in an urban-like environment.

Comment: The presentation of the results is classically similar to a point source reconstruction study which do not highlight any significant contribution related to optimal networking.

Reply: *In the present study***,** *the obtained optimal networks were analyzed qualitatively and quantitatively for all the trials of the MUST field experiment. The dispersion of the sensors in the urban-like environment was critically analyzed according to the source position and the meteorological situation. A fine analysis is performed to highlight the common structures (Skeleton) in the optimal networks. Also, a posteriori study is realized in order to evaluate the performance of the optimal networks. For this, the errors in source parameters estimation are compared with the errors obtained from the original network which leads to the important conclusions in networks size reduction in the framework of source reconstruction in an urban environment. As the applicability of the obtained monitoring networks is validated and analyzed by estimating the source parameters from the concentration measurements from the optimal networks, it is obvious to present and analyzed the source reconstruction results and compare these with from the previous study. We do not agree with Dr. Singh's point that this study does not highlight any significant contribution related to optimal networking. In fact, using the proposed methodology, we were accurately able to estimate the source parameters using the measurements only from 1/4th and 1/3rd sensors with approximately similar accuracy compare to the network of original number of sensors. This is a significant contribution that reduces the number of sensors in an urban-like environment and without compromising the ability of the network with a minimal number of sensors to estimate an unknown source.*

Comment: The application of renormalized inversion and SA methodology in optimizing receptors are associated with several issues which are not clarified in the text.

Reply: *As mentioned in the abstract and in the text the renormalized inversion method, the SA and the CFD model were coupled to obtain the optimized network of the receptors and the related issues were partially presented when the methodology of the networks optimization was presented for an urban-like environment. We have more clarified these issues in the updated version of the manuscript.*

Comment: Besides, there are several examples of uncleared and overstated sentences, misinterpretation of mathematics, poor description of results and methodology.

Reply: *Unfortunately, we cannot answer to a not given examples. Can you please indicate the "uncleared and overstated sentences" and the ''misinterpretation of mathematics''? However, we will carefully read again and correct the text in the updated manuscript for such examples (if any).*

Comment: Overall, it needs to be justified that what is the significant outcome of this study and how their approach of determining optimal network, which is biased towards measurements, is justified in a general framework?.

Reply: *As clarified before (see the first reply), this study is carried out in the framework of the cases (3) and (a). We do not study all the envisaged cases. It is clear that the problem of sensors network optimization is not trivial and need to be solved according to a given configuration. We remind that in this study we provide an answer to the specific operational need for which it is necessary to deploy sensors in emergency situations where the meteorological conditions are known in real time and some information about the measurements are available. We explain more: for example, in an industrial site the area where an eventual source can be located is known. Consequently, the source is roughly localized and the optimized network is deployed to refine the estimation of the source position which helps to repair the installation. A second concrete case concerns the estimation of the intensity of hazardous accidental release. This data (i.e. intensity of the source) is primordial for following and/or for predicting the evolution of the accidental plume. In such specific case, it is judicious to be based on the scenarios which justify the use of concentrations in optimal design. For more clarification we cite some example of works based on these scenarios (i.e. a priori information are available) where the measurements were used in the optimal design of the monitoring networks:*

- *(Ma et al 2013): Comparison and improvements of optimization methods for gas emission source identification.*
- *(Mason et Bohlin, 1995): Network optimization of a radionuclide monitoring system for the comprehensive nuclear test ban treaty.*
- *(Berry et al, 2006-a): A facility location approach to sensor placement optimization.*
- *(Watson J-P et al, 2004): A multiple-objective analysis of sensor placement optimization in water networks.*
- *(Krause et al, 2008) Efficient Sensor Placement Optimization for Securing Large Water Distribution Networks.*
- *(Hamel et al, 2010): Sensor Placement for Urban Homeland Security Applications.*
- *(Abida et Bocquet, 2009): Targeting of observations for accidental atmospheric release monitoring.*

Also, we can find in the literature some works of sensors networks optimization based on <u>error cost function (error objective function) similar to the optimality criterion that we proposed in our study:</u>

- *(Abida et al, 2008): Design of a network over France in case of a radiological accidental release.*
- *(Saunier et al, 2009): Model reduction via principal component truncation for the optimal design of atmospheric monitoring networks.*
- *(Jiang et al, 2007): Optimization of mobile radioactivity monitoring networks.*

This study shows that it is possible to reconstruct a source of atmospheric emissions with a limited number of concentration measurements and presents a methodology for selecting the 'best' sensors positions based on an optimality criterion and by coupling an optimization algorithm an inversion method and a CFD model that include the complexity of an urban domain. This study presents a practical method for managing realistic situations. In an area of interest, it is not possible to place the sensors anywhere. This study presents an investigation of the measurements vector used in the inverse problems.

General Comments:

Comment 1. In network optimization problem, finding an optimal rearrangement of a set of receptors and then, their evaluation for source estimation are two independent set of problems. The determination of optimal rearrangement should be performed independent of knowledge of measurements and it must contain available maximum information in the domain regarding observability of emissions. The second problem regarding evaluation of source retrieval should be carried out as a next step to validate the efficiency of such networks in the presence of random model-measurement errors. In this study, the two set of problems are mixed and arrangement of network is determined given the knowledge of measurements which is a biased choice of receptors. In addition, the study does not discuss any criterion which could quantify the information in a particular design or impact of model-measurement errors on the chosen network.

Reply: *We agree with Dr. Singh's remarks that in a network optimization problem, finding an optimal rearrangement of a set of receptors and then, their evaluation for source estimation are two independent set of problems. In fact, we also followed the same procedure. The network optimization problem was independently presented and performed before any evaluation by estimating the source parameters using the measurements from the sensors from the obtained optimal network. However, since the optimization methodology utilizes some concepts (not the source estimation part) from the renormalization inversion methodology, we presented it after the source estimation methodology. As also explained in the manuscript and more clearly in the updated version, the network optimization problem is completely independent of the source estimation evaluation. It is very clearly explained in the flow diagram of the methodology in Figure 2 and shows that source was estimated only when we obtained the optimal monitoring network. In this work, the first step consists to find the best configuration of a limited set of sensors using the meteorological data, the sensors positions on the instrumented area, a CFD technique and the concentration observations. The second step consists to evaluate a posteriori the performance of the optimal networks in comparison with the original network used in the MUST field experiment.*

The problem of optimal design of sensors networks for source reconstruction can be performed (i) without a priori information or (ii) with a priori information of the source (such us its position, intensity, etc.) and the observations (i.e. measured pollutant concentrations) can be used in the optimization process see as examples (Ma et al, 2014).

In a case when the source is considered completely unknown (as for an example in a terrorist attack) the challenge is to design a network able to reconstruct an eventual source regardless of its position and intensity. Thus a specific cost function could be defined in order to assure the optimal design and the concept of information can be used. The Ph.D. thesis of Kouichi (2017) and Kouichi et al. (2016) was inspired by this concept for defining the entropic criterion based on the renormalization method in order to estimate the best arrangement of the sensors for source characterization regardless its intensity and position. This work is already a subject of a publication that we realized.

In a case when some knowledge about the source is available we remind as example on industrial sites the 'danger zone' were the source can be located is completely known (storage tank of hazardous products, network of pipelines, etc.) for this reason works of optimization can be conducted based on scenarios for witch a priori information on the source was utilized (another example in specific situation of accidental release the position of the source is known (observed in the site) and the need is to estimate its intensity in order to estimate the dispersed quantities of a hazardous agent this can help to predict the *evolution of the accidental plume or to determine the contaminated area or to estimate the quantities inhaled by the personals exposed on site, etc.*

Concentrations measurements can routinely be available from an already existing large monitoring network. In this study, we utilized these concentration measurements to reduce the size of a large network. The updated version of the manuscript also discusses a posteriori error analysis of the source reconstruction based on the random measurements errors from an obtained monitoring network.

Comment 2. Throughout the text, authors have mentioned the keyword "optimal network". A big question here, is how to prove that a particular design is optimal?. This requires rather mathematical or statistical arguments / proofs to support the fact that a design is optimal. This can not be shown by showing source retrieval which is nothing but just the estimation of 3 parameters (location, (x, y) and strength q).

Reply: *Throughout the text we mentioned that there is no guarantee in the convergence of the SA and we confirmed (based on the adequate bibliographical references) that the obtained network can be the optimal or the near-optimal one. This complex combinatorial optimization approach retained a big attention in the literature and the SA is selected following the recommendations from more than one works of networks optimization in the framework of the atmospheric dispersion context (Abida et al, 2008; Abida et Bocquet, 2009; Jiang et al, 2007; etc.). Nevertheless, before utilizing the probabilistic algorithm SA, we tested its performance in comparison with the Genetic Algorithm GA of evolutionary research technic (Kouichi, 2017). Concerning the statistical study after the achievement of the optimization, we plan to perform this investigation as continuity of this first study.*

Comment 3. A big limitation of this approach is the subjectivity and biasness in the methodology and their dependence on the measurements. The optimality of the reduced set of receptors is shown based on the accuracy of the point source retrieval which is not relevant. The good retrieval results with presumed lesser number of receptors are not surprising since their chosen cost function depends on the measurement's values which always force the SA algorithm to choose the receptor locations with good model measurement accuracy. They completely ignored the fact that their network design criterion should be independent and prior to the knowledge of measurements, which is one of the big limitations. To be precise, the optimization methodology utilizes the same cost function for both the tasks: (i) Identifying a reduced set of receptors and (ii) retrieving the point source parameters. The cost function utilizes the actual measurements and measures the deviations between measured and predicted concentrations at the chosen set of receptors. The iterative SA algorithm tries to minimize this cost function, which means it selects the receptors with good model-measurement accuracy, i.e. which are closer to the measurements. This will eventually results in good retrieval depending on the model error. This clarifies the fact that the choice of receptors is always subjective to the model-measurement accuracy and will vary in case of perturbation in the model measurement variables. Thus, this is a poor approach and always biased towards model-measurement accuracy which do not signify the objective of optimization of receptors. The optimization of receptors should have performed independent and prior to the knowledge of measurements, which is not done here.

Reply: *This comment is similar to the comment n°1 and some evoked points in the introduction so we conserve the same responses. We hope that the clarification that we presented before help for best understanding the aim and the approach of this study.*

Comment 4. The study do not provide any insights / discussion on systems observability while remaining ill-posed, quantification of information gain or loss during optimization of the network, statistical or mathematical criterion leading to network optimization and sensitivity of the network design with respect to the perturbation in the model-measurement variables. Also, the study do not mention any optimality criterion, design of experiment or information theory criterion.

Reply: *The sensitivity of the network design with respect to the perturbation in the model-measurement variables is studied a posteriori and discussed in the revised version according to the recommendation of the Referee#2. Concerning the optimality criterion and the information theory, we remind as we mentioned before (reply for comment 1) that the entropic criterion for optimal monitoring networks is defined by Kouichi (2017) and is the subject of another publication. We hope that the clarification that we presented before, especially the framework and the challenge of this study is now clear (mobile networks, with a priori information, etc.)*

Comment 5. Another issue with the methodology is that the SA algorithm may not converge always to the same set of reduced receptors. More often, there is high probability that the reduced set will change in every repeated simulation since the number of possible combinations are really high. In this case, how do you guarantee the optimality of design?. Also, the authors never compared between various such different sets corresponding to same trials as how they are varying or what are the differentiation between them. It seems that the authors just choose the arrangement with least reconstruction error which is not logical.

Reply: *This comment is similar to the comment n°2 and some evoked points in the introduction so we conserve the same responses that we clarified before.*

Comment 6. If the objective was simply to have a reduced set of network where model measurement errors are minimum (which is done here), why authors just did not select those locations where model predictions are matching with measurements?. This could be done simply by comparing model predictions and measurements instead of a massive SA computation. Based on the proposed approach, this can not be called an optimization of the monitoring network.

Reply: *Selecting the locations where model predictions are matching with measurements doesn't guarantee a 'best' estimation of the source parameters (inverse problem and direct problem are completely different). Effectively, this is one of the important results of this study. As we used a data assimilation approach, the best network is obtained for the best reproduction of the observations (i.e. correspond to the minimal quadratic distance between the modeled and the measured concentrations). Also, as stated by Dr. Singh about the network based on the matching of direct model prediction with measurements, the direct model also required the knowledge of the exact source parameters and this information may not be available in general. However, in this study, we utilized only the concentration measurements and not the source parameters to obtain the monitoring networks.*

Comment 7. The proposed approach also raises questions regarding the efficiency of the network in case of perturbed model-measurement fields/variables. Also, the retrieved parameters are highly sensitive toward the design of their network which raise further questions regarding the efficiency of the chosen network. The optimized choice of network will always be subjective with respect to the wind variability, model, model errors and measurements. In trials, where model does not perform well, the error will always be high, for example see in trials 2. This will raise the issue of failure of their monitoring networks in identifying correctly the emissions in case of large model errors. This is why the arrangement of the receptors vary in all the trials, even when in some trials, the wind conditions are approximately similar.

Reply: *This study presents our first attempt of the sensors networks optimization for the reconstruction of releases source in urban domains. The door are still open for continuity in order to integrate the effect of meteorological conditions variability or to integrate the influence of the model's errors. Nevertheless, following the recommendation of the Referee#2, the effect of random measurement errors is now integrated into the analyses of the performance of the optimal network. Some limitations of this work are also included in the updated version of the manuscript. It is not always true as Dr. Singh commented that in trials, where the model does not perform well, the error will always be high, for example, see in trials 2. In trial 2, the predicted concentrations from direct model were in good agreement with the observations (NMSE = 0.17, Correlation coefficient = 0.95, Index of Agreement = 0.97) (Kumar et al., 2015a). Even by utilizing the concentration measurements from all 40 sensors in source estimation, the retrieval error was large in this trial 2 (Kumar et al., 2015b). Also, all problems of the optimizing the network, e.g., networks without using concentration measurements, one single network for all meteorological conditions, etc. cannot be deal in a single study. The optimal networks dealing with some of these problems were partially presented in the Ph.D. thesis of Kouichi (2017) and will be presented in separate publications.*

Comment 8. The study also discusses about weights which they, later, referred as visibility functions highlighting prior informations regarding emissions. However, authors never mention "why they could not determine a criterion based on just visibility weight functions"? Which could be far relevant and independent to the measurements.

Reply: *The method that we described to assure the optimization is not unique, it is possible to use the visibility as optimality criterion and it is a different approach. In any case, we mentioned that the renormalized errors criterion is the unique cost function that can be used to assure the design in such problem configuration. The optimization approach only based on the visibility weight function was also performed as another research problem in the Ph.D. thesis of Kouichi (2017). <u>Dr. Singh is well aware of this study and corresponding partial results as he was also present in the final Ph.D. viva presentation of Hamza Kouichi</u>.*

Comment 9. It is not clear why they could not find a common optimal network which could work in all the trials for point source retrieval?. The original network of 40 receptors was already working in all the trials irrespective of model errors and varying meteorological conditions. It is useless to propose different configurations based on different meteorological conditions since meteorology can never be constant in a real scenario. The different configurations for different trials again highlight subjectivity of their approach. Thus, the study do not bring any significant outcome regarding the optimization of receptors.

Reply: *As we clarified before (see first reply in page 2 / case of permanent static network), finding a common optimal network which could work in all the trials is a different optimization problem, also an adequate optimality criterion (entropic criterion extended for several meteorological situations) is defined by Kouichi (2017). <u>Dr. Singh is well aware of this study progress and corresponding partial results as he was also present in the final PhD</u>*

viva presentation of Dr. Hamza Kouichi. *We remind, this study is specific to emergency situations where the meteorological conditions can be known in real time and don't vary significantly (it is assumed as stationary because the problem of optimization in an urban environment is very complex and this is our first tentative in this framework).*

Comment 10. How do you describe physical features and efficiency or quality of the reduced configuration?. This is never mentioned in the results and discussion. The discussion mainly involves only source retrieval.

Reply: *We analyzed qualitatively (structures of the optimal networks in the instrumented area) and quantitatively (errors in source reconstruction) and the results showed that no trend is obvious thus proves that the problem of sensors networks optimization in urban environment is not trivial also the reduction of an original network achieved successfully and the performance for source reconstruction is maintained.*

Comment 11. Why their optimization always results in finding most of the sensors (5-6 detectors in the reduced configuration) close to the source location? It was never explained in the text. Does your optimized choice of receptors depends significantly on the receptors closer to the source location?. If yes, then what is use of optimizing since you will never know the source in accidental scenarios?

Reply: *Most of the sensors are selected by the SA close to the source location and this tendency is logical because these sensors make the area around the real source well visible from the network, nevertheless, this doesn't guarantee a correct reconstruction of the source. As examined by Kouichi (2017), in some cases a limited number of sensors close to the source are not enough also adding sensors to a 'key configuration' don't improve the precision in source parameters estimation thus prove that the reduction of the number of sensors is justified. We remind that this study is for a specific need where a priori information (i.e. the measurements) is available and the networks are optimized to be deployed in emergency situations.*

Comment 12. Why signal to noise ratio is not shown for all the reduced configurations? and it should be compared with the original network?

Reply: *Can you please clarify what do you mean by 'signal to noise ratio' in this context?*

Comment 13. The authors have simply described the errors in retrieving the location and intensity of the source. The responsible reasons behind it were never explained?. This shows that authors are just interpreting the retrieval rather than really analyzing the results.

Reply: *This comment is similar to the comment n°10 so we conserve the same responses.*

Comment 14. What is the role of weight function in your reduced configuration?. Does it have any effect on the systems observability and how it do affect your retrieval?

Reply: *Fundamentally, the role of the weight function in the renormalized data assimilation is minimizing the over interpretation of the observation, concerning the optimal networks no evident trend is relieved this confirm the complexity of such problem.*

Comment 15. Why did you describe vectors on the figures of the source retrieval?. While it seems that you are retrieving source parameters in a weighted least-squares framework?. It was never explained in the results that what is the impact of reducing the receptors on the retrieved general source vector?.

Reply: *The source vector* ***s*** *is not described separately but analyzed with the visibility field obtained by the optimal networks and for each trial of the MUST experiment. The goal is to assure a qualitative examination and to validate the fact that the optimal network covers correctly the source position. Also to confirm that in the monitored area only one punctual source is detected, in the figures by analyzing the level in the source vector we confirm that the maximum is unique so the estimated source after the reduction of the original network size is physically coherent.*

Comment 16. A general choice of using a weight matrix in a least-squares methodology is measurement error covariance matrix. Authors did not justify how could they utilize matrix Hw as an alternative to measurement covariance matrix?. In addition, the Hw matrix is not a diagonal matrix which means that using Hw as a weight matrix will induce unphysical correlations among receptors which could be false as well. Did you analyze their impact on source retrieval?, If not, then why and how could you use them directly? Perhaps, you could assume an unity matrix. If not, why?

Reply: *As explained by Issartel et al. (2012), classically, the least squares are weighted using the covariance matrix (Hw) of the measurement errors. However, in practice, this matrix cannot be determined for the prevailing part of these errors arising from the limited representativity of the dispersion model. Issartel et al. (2012) proposed an alternative weighting based on a matrix Hw, that is related to a unified approach of the parametric and assimilative inverse problems corresponding, respectively, to the identification of the point of emission or estimation of the distributed emissions. The weighting was shown to optimize the resolution and numerical stability of the inversion (Issartel et al., 2012). The importance of the most common monitoring networks, with point detectors at various locations, is stressed as a misleading singular case. As discussed by Issartel et al. (2012), it is possible to understand a drawback of two classical choices of Hw as the identity matrix, associated with the ordinary norm, or as the diagonal covariance matrix of noise supposed to be uncorrelated in the various measurements. The justification to utilize the matrix Hw is proposed and given in Issartel et al. (2012). A brief discussion of the justification is presented in the revised version.*

Comment 17. Another issue is with the presentation of the methodology. The study begins by posing an under-determined inverse problem of estimating state of emissions while their objective was to optimize a reduced set configuration for point source retrieval which is an overdetermined inverse problem. Why authors did not begin by directly posing the over-determined problem of point source retrieval?. Why they have presented unnecessary details regarding more general inverse problem of estimation emission state if it was not their objective?. The presented details were already published by several researchers in the literature. Further, authors again formulate the point source retrieval problem in a weighted least-squares sense. Why?. Why two different methods were presented for the same problem?.

Reply: *Before presenting the optimization methodology a brief mathematical formulation of the renormalisation technique is presented for a simple reason that we cannot define the optimality criterion without presenting its origin and its physical signification. If we present* *directly the adequate cost function (i.e. normalized errors) this cannot be appropriate for readers that don't have any information about the renormalisation method. Concerning the 'detail' of point source estimation simply because for the quantitative analyses (i.e. performance in source parameters estimation) we use this method so it is logical to present this 'detail'. However, as suggested, this part is reduced subsequently in the updated manuscript.*

Comment 18. Why do you need to compute a general vector s of state of emissions?. The objective was just to estimate point source parameters which could be estimated with the weighted / non-weighted least-squares method?. Please clarify?.

Reply: *This comment is similar to the comment n°15 so we conserve the same responses.*

Comment 19. Again, in the results, figures highlights distribution of weights and vector s which was never related to their monitoring network optimization. Their presentation confuses the overall objective of the study. Do you propose an optimal design for point source retrieval or a general source retrieval?. The figures related to weights are never explained as why they were needed? or what information do they provide related to the monitoring arrangement?. The given explanation is just copy-paste from previous papers of the authors.

Reply: *This comment is similar to the comment n°15 & n°18 so we conserve the same responses. However, the figures related to the visibility function are discussed with respect to the corresponding optimal monitoring networks in the updated version of the manuscript.*

Comment 20. Why authors did not compare the weights in comparison to their weights corresponding to the original receptors?.

Reply: *We compared the performance of the optimal networks in comparison to the original network this implicitly and indirectly inadequate the role of the weights for each network.*

Comment 21. Another issue is also related to the common base network among the 10 and 13 sensors network. Why their strong base network involves only 7 receptors? In general, the 10 sensors networks should be a subset of the 13 sensor network, if not then why?. Please clarify?. It is also surprising that in some trials the common base network involves only 3 sensors. This is unusual having so much variation in having common base sensors among 10 and 13 sensor network in trials. The authors should provide the reasoning behind?, not just mentioning the results.

Reply: *The analyses of the common structures (Skeleton) in the optimal networks confirm that the solution is not unique so more than one network can lead to a good estimation of the source parameters. This result is very important and is in coherence with the works of Kovalets et al. (2011) and Efthimiou et al. (2017) that confirmed for the same experimental data the best source reconstruction using 10 sensors is possible for 5% or 10% among a significative set of randomly networks.*

<u>Specific comments:</u>

1. Abstract, Page 1, line 7. The sentence "The optimal networks in the MUST urban regions enabled ...". Rephrase the sentence. How could an optimal network enable a reduction?. I would like to mention again that the reduced set of receptors were never proved optimal.

Reply: *The sentence is rephrased for more clarity in the updated version. However, another part of this comment is similar to the general comments n°2 & 5 and some evoked points in the introduction so we conserve the same responses that we clarified before.*

2. Abstract, Page 1, line 11. The sentence "This study presents first application of the renormalization data assimilation approach for the optimal network design : : :.." is overstated and wrong. I could not find where and how did you apply renormalize data assimilation for optimal network design. Renormalize assimilation is only for retrieving the source parameters. I do not see in the text, how it could retrieve the reduced set of receptors. Also, you have interpreted a least-squares framework without justifying their inherent equivalence and choice of parameters with respect to the renormalization. Why?.

Reply: *We modified this sentence in the updated version, however, the later part of this comment is similar to more than one comments and some evoked points in the introduction so we conserve the same responses. We hope that after the clarification, the aim and the presented methodology are now clear. A brief discussion about the justification of the weighted least-squares with respect to the renormalization framework is presented in the revised version.*

3. Page 1, line 18, the sentence "However, pre-deployment of these limited number of sensors : : :..". Please clarify, how could a pre-deployment of sensors helps to achieve maximum information from set of noisy concentration measurements. The objective of pre-deployment of sensors is to have maximum a priori information regarding state of emission and to correctly capture the data while extracting and utilizing information from the data is the final task of data fusion techniques.

Reply: *This comment is similar to more than one comment and some evoked points in the introduction so we conserve the same responses.*

4. Page 2, line 2. The sentence "detection of an unknown continuous point source's parameters ..." is wrong. How could you detect point source parameters? They are rather retrieved or estimated.

Reply: *We agree with this comment and accordingly, the sentence is modified.*

5. Page 2, line 12. See the sentence "The establishment of an optimal network requires...". Why do you think that for an optimal network it requires availability of concentration measurements?. Please justify? Measurements may be required for the evaluation or validation but for establishment a network can be made with the meteorology and dispersion model.

Reply: *This comment is similar to more than one comment and some evoked points in the introduction so we conserve the same responses. This point was explained earlier in detail.*

6. Page 2, line 20, See the sentence "This approach includes the geometric and flow complexity inherent : : :..". I do not think if there is any inverse approach which includes such things for optimization process. The flow variables are accounted through the model, perhaps in the inverse approach in the form of sensitivities which is also derived from adjoint model. All the STE approach can include such information from model.

Reply: *The approach term written here doesn't mean to refer the inversion or STE approach only. It refers to the whole methodological approach to optimize the network by coupling the optimization techniques, inverse tracers transport modeling, and Computational Fluid Dynamics. However, it is modified to avoid any confusion.*

7. Page 2, line 26. What is "regularized norm square". I do not think Sharan et al., 2012 have included such terms.

Reply: *The sentence is modified.*

8. Page 3, lines 3-5. Issartel, 2005, Sharan et al., 2009, 2012 and Kumar et al., 2015b, do not discuss any iterative algorithm to minimize the difference between observed and modeled concentration.

Reply: *The sentence is modified.*

9. Page 3, line 8, "does not required". Please correct the sentence.

Reply: *Corrected.*

10. Page 3, lines 16-17, Kumar et al. (2015b, 2016) do not provide any extension to renormalized inversion. It was just an application with CFD model.

Reply: *Modified.*

11. Page 3, lines 22-29. The authors defined the objective to determine optimal network but never achieved. In line 23, "A methodology was proposed : : :: : :.". If the objective was to better characterize the source, why one need to reduce the number of receptors. The reduction of receptors simply refers to the reduction of information regarding the observability of state of emissions. In line 26, "For this purpose : : :., but with comparable information". Where do you show in the manuscript that the reduced information is comparable to the original network. In line 27, "This work explores with two requirements : : :...", What does it mean, there is no movement of sensors. You have performed only selection of sensors.

Reply: *This comment is similar to more than one comment and some evoked points in the introduction so we conserve the same responses.*

12. Page 4, line 2, please correct "concentrations measurements".

Reply: *Corrected.*

13. Page 4, line 4, please correct "an horizontal plane".

Reply: *Corrected.*

14. Page 4, lines 8-10, The sentence "This study deals with linear relationship, as except from the nonlinear chemical reactions : : :.." is wrong. Most of these process are nonlinear in your case due to complex flow structures.

Reply: *This statement was based on the cited reference and we will verify it again and remove/correct it accordingly.*

15. Page 4, line 26, citing Kumar et al., 2016 is not appropriate. Please cite appropriate reference.

Reply: *We will check and correct the appropriate reference if needed.*

16. Page 4, lines 28-30, I understand that the inverse solution from Eq. (2) will lead to peaks at the grid cells coinciding with the measurement cells. This is obvious since the sensitivity matrix has peaks at the measurement cells which are reflected in the inverse solution. However, the difficult part to understand is "why do you call these large values of sensitivities at measurement cells an artificial information? Or a virtual/unphysical reality?". The peak at measurement cells is obvious since the concentration is always maximum at source location and in adjoint computations, you have replaced your measurement cells as source. Please clarify.

Reply: *These points were already clarified in many papers of Dr. J.-P. Issartel (main developer of the Renormalization inversion theory) and also in some other papers of his coauthors including Dr. Singh. In fact, this was one of the main force to the development of the renormalization inversion technique for source estimations which Dr. Singh has also used a lot in his papers.*

17. Page 5, line 5, Why do you think that normalizing peaks in the sensitivity matrix with weights will cure the peak problem. I mean, even if you normalize peaks (infinitely large value) by some nonzero weight values, it will not change anything.

Reply: *We don't understand this comment can you please more clarify? However, these points were already clarified in most of the papers related to the renormalization inversion technique.*

18. Page 5, line 9, citing Kumar et al., 2016 is not appropriate. Please cite appropriate reference.

Reply: *We will check and correct the appropriate reference if needed*

19. Page 6, line 3, "but with comparable information". It is never done in the study.

Reply: *What do you mean by "It is never done in this study"? In the evaluation of the optimized networks, we have compared the source estimation performances of the obtained optimal networks of a reduced number of sensors with the original network of 40 sensors. The obtained optimal networks with reduced sensors provided comparable estimates of the source parameters with the estimates obtained from the original network of 40 sensors.*

20. Page 6, line 4, "delivers maximum of the information". It is never shown in the study.

Reply: *It is a statement that refers to define one of the objectives of an optimized monitoring network to deliver a maximum of the information in respect to the source estimation from a reduced number of sensors in an optimized network. We do not think any wrong in this sentence.*

21. Page 6, line 11, why cost function is defined according to Hw norm. Please clarify?.

Reply: *Because our approach is based on the renormalized data assimilation method as an inverse technique. It was explained in several studies, originally discussed in a study by Issartel et al. (2012). It is more clarified in the updated version of the manuscript.*

22. Page 6, line 12. Check sentence "As the cost function is convex, its minimum value must correspond to the maximum intensity of the source". WHY?. Please clarify?. The intensity of source here is q. Check your mathematical expressions. You will obtain an estimate of q for each location vector x. In such case, the maximum value of q in the domain may go to infinity in case where weights w are very small or zero. It is not necessary that the maximum value of q will occur at the minimum of the cost function or at the source location.

Reply: *We agree with Dr. Singh's remark about the cost function which was mistakenly stated that way. This sentence is removed/modified from/in the updated version of the manuscript as it doesn't affect the subsequent part of the methodology.*

23. Page 6, line 15. This is not clear how you can utilize matrix H_w in place of measurement error covariance matrix in Eq. (9). This is not obvious. Justify?.

Reply: *As it was explained in several studies, originally discussed in a study by Issartel et al. (2012), it is more clarified in the updated version of the manuscript.*

24. Page 6, line 16, why two notations q and q0 (section 2.4) are utilized for the same representation?

Reply: *Thank you for pointed it out. We have corrected it to the same symbol throughout the manuscript.*

25. Page 6, line 19, "conditions of maximum intensity: : :.". It seems that authors have difficulties in understanding mathematics. Why equating first order derivative to zero will give maximum intensity?

Reply: *The sentence is corrected. It is just a simple derivative test of a function to find its critical points that determines whether each point is a local maximum, a local minimum, or a saddle point. Here, equating the first order derivative to zero leads to an estimate of the source intensity.*

26. Page 6, line 25, The expression for equation (13) is wrong. Please correct it.

Reply: *Corrected.*

27. Page 6, line 26. The mathematical expression is wrong.

Reply: *It seems to be correct; however, we will verify it again and modify if needed.*

28. Page 6, line 27. How do you guarantee the global minimum in SA algorithm?.

Reply: *This comment is repeated again and similar to more than one comments and some evoked points in the introduction so we conserve the same responses.*

29. Page 7, line 16, "average of the difference of the cost functions calculated for a large number of cases". How did you compute it?

Reply: *This is for estimating the starting 'temperature', the procedure consists in generating a set of random networks of the same size than in evaluating the quality of each network using the renormalization algorithm.*

30. Page 7, line 19, "An equilibrium is reached : : :..". This means that the SA algorithm stops when cost function becomes constant. Then how do you prove global minimum?

Reply: *This comment is similar to more than one comments and some evoked points in the introduction so we conserve the same responses.*

31. In combinatorial optimization problem, it is not necessary that SA will provide the same solution or same set of receptors as the converged solution. In this case, how did you choose the solution?.

Reply: *This comment is similar to more than one comments and some evoked points in the introduction so we conserve the same responses. All the details about the SA and haw it is employed in this context are also available in Kouichi (2017).*

32. Page 8, step 2 and step 3 show that the choice of receptors depends on the measurements. Thus, there is no optimality in network. The authors have simply chosen the reduced set of receptors based on good retrieval results which is biased.

Reply: *The question is repeated again and the answers to these points are already given to his previous comments.*

33. Page 9, lines 8-11. These are not clear. What do you mean by near-optimal network?. What are the conditions for "near overall optimum condition".

Reply: *As explained before, all these details are available in the cited references in the literature.*

34. Page 11, line 11, "The network optimization process : : :..". This shows that the choice of receptors are biased towards the model-measurement accuracy.

Reply: *Again the same question is repeated and so we conserve the same responses as given earlier.*

35. Why the configuration of networks should vary based on meteorological stability conditions.

Reply: *This is evident because the arrangement of the sensors in the monitored area should be according to the wind direction for example. It is clear that we cannot place sensors in regions were no measurements will be collected. We remind that the objective of this study is not to optimize a permanent static network.*

36. Page 12, lines 8-9. "These results exhibit that the SA : : :..". How it prove optimality of monitoring network?

Reply: *The answer is already given to this question as this comment is similar to more than one comment and some points in the introduction.*

37. Page 12, line 19. "were observed independently of the number of sensors". Why?. Please clarify?.

Reply: *This is showed in Table 2. However, the sentence is modified to avoid any confusion.*

38. Page 12, line 20, “larger location errors do not : : :.”. Why?. Please clarify?

Reply: *This is noted in the results.*

39. Page 12, line 23, “a large number of sensors are close to the source positions ..”. Why so?. Please justify?.

Reply: *This is noted in the qualitative analyses. This point is already clarified in response to a similar earlier comment.*

40. Page 12, line 29, “visibility functions have significant levels : : :..”. What does this mean?.

Reply: *This is noted in the qualitative analyses please see figures 4 & S2.*

41. Page 13, line 6, “increase in the number of sensors in a network has little influence on the accuracy: : :.” Why? Please clarify?

Reply: *This is clear in the text because by adding sensors in a performance network can more add measurements and model errors in the methodology which may affect the estimation of the parameters of the source.*

42. Page 13, lines 8-10, “In some trials, it was also noted : : :..not necessary benefial.” How could you justify this?. In fact, how did you evaluate if information added by a sensor is fruitful or not? If just based on accuracy of source retrieval, then it is illogical? If an information added by a new sensor is not beneficial then why it should increase the location error?. Also, how location error may decrease with decreasing the number of sensors? You can say this just because you are looking at source retrieval estimates. However, reducing the receptors will make the source retrieval unstable and more sensitive to the noise.

Reply: *We tried to explain these points in this section of the manuscript as it was observed in some trials. The distance of an estimated source to real source was observed to decreases with an increase in sensors number and also with the decrease number of sensors in some other cases. At this moment, we do not have a theoretical explanation for this behavior. However, it is also logical that increasing the number of the sensors after a number may not always provide the best estimation because with addition of the more no. of sensors, we also add more model and measurements errors in the estimation process. These errors may affect the source estimation results in some trials. As pointed out by Dr. Singh, reducing the receptors will make the source retrieval unstable and more sensitive to the noise, this problem may also require a theoretical justification of the minimum number of sensors needed for source estimation. And it is beyond the scope of this study. However, these limitations are now explained in the updated manuscript.*

43. Page 13, line 17, What do you mean by “: : : diversity of structures independently of the number of sensors.” You computation is based on fixed number of sensors and there is no discussion of diversity. However, in the following explanation, this is not understandable that why you have different number of common networks in different trials?. It seems that optimized choice of receptors is not really optimized. Otherwise, why in some trials (1, 11), only 3 sensors are found as a common base?. Also, even having 7 receptors as common in 10 and 13 sensor arrangement can not be called a strong common base. There is no explanation

why all the 10 sensors are not subset of 13 sensor network. If, it was really optimized that it must have been. If not so, then please explain why?

Reply: *This comment is similar to the major comments n°21 so we reserve the same responses that we clarified before.*

44. Page 13, line 22, "The performances do not systematically converge independently to the size of the networks". What does it mean and why it does not converge?. Further, it is mentioned that in trial 1, 13 sensor network leads better performance than a 10 sensors network and algorithm leading to near global optimum is contained in the 13 sensor network. This really proves that fact that you choice of receptors is biased by your source retrieval which is not the objective of an optimal network.

Reply: *This comment is similar to more than one comment and some evoked points in the introduction so we conserve the same responses. However, we wish to point out again that the choice of the receptors were not determined based on the source estimation. These optimal sensor locations were independently estimated based on the concentration measurements, adjoint functions, and SA algorithm. The source estimation is performed only to validate the performance of the obtained optimal networks.*

45. Page 13, line 27. Why there is no common trend in skeleton network observed in several trials?. There must be at least with similar flow conditions. If not, justify?

Reply: *This comment is similar to more than one comment so we conserve the same responses.*

46. Page 13, line 29, "optimal networks can satisfy conditions of a near overall optimum (to be minimized)". What are the near overall optimum conditions?. If you are referring "minimization of cost function". This is a wrong approach.

Reply: *This comment is also similar to more than one comment. Throughout the text we mentioned that there is no guarantee in the convergence of the SA and we confirmed (based on the adequate bibliographical references) that the obtained network can be the optimal or the near-optimal one. This complex combinatorial optimization approach retained a big attention in the literature and the SA is selected following the recommendations from more than one works of networks optimization in the framework of the atmospheric dispersion context (Abida et al, 2008; Abida et Bocquet, 2009; Jiang et al, 2007; etc.). Nevertheless, before utilizing the probabilistic algorithm SA, we tested its performance in comparison with the Genetic Algorithm GA of evolutionary research technic (Kouichi, 2017).*

References

Abida, R., Bocquet, M., Vercauteren, N., Isnard, O., (2008). Design of a monitoring network over france in case of a radiological accidental release. Atmospheric Environment, 42, 5205–5219, doi: 10.1016/j.atmosenv.2008.02.065.

Abida, R, et Bocquet, M., (2009). Targeting of observations for accidental atmospheric release monitoring. Atmospheric Environment, 43, 6312–6327, doi: 10.1016/j.atmosenv. 2009.09.029.

Ainslie, B., Reuten, C., Steyn, D. G., Le, N. D., & Zidek, J. V. (2009). Application of an entropy-based Bayesian optimization technique to the redesign of an existing monitoring network for single air pollutants. Journal of environmental management, 90(8), 2715-2729.

Berry, J., Hart, W., Phillips, C. A., and Watson, J. P., (2006-a). A facility location approach to sensor placement optimization. 8th Annual Symp.on Water Distribution Systems Analysis, Cincinnati, Ohio, Environmental and Water Resources Institute of ASCE (EWRI of ASCE), New York.

Chen Q, Wu W, Blanckaert K, Ma J, Huang G. Optimization of water quality monitoring network in a large river by combining measurements, a numerical model and matter-element analyses. J Environ Manag, 2012;110: 116–124. doi: 10.1016/j.jenvman.2012.05.024)

Hamel, D., Chwastek, M., Garcia, M., Farouk, B., Kam, M., Dandekar, K. R., (2010). SensorPlacement for Urban Homeland Security Applications. International Journal of Distributed Sensor Networks, vol. 2010, Article ID 859263, p15.

Issartel, J.-P., Sharan, M., and Modani, M.: An inversion technique to retrieve the source of a tracer with an application to synthetic satellite measurements, Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, 463, 2863–2886, https://doi.org/10.1098/rspa.2007.1877, http://rspa.royalsocietypublishing.org/content/463/2087/2863.abstract, 2007.

Issartel, J-P., Sharan, M., Singh, S.K., (2012). Identification of a point of release by use of optimally weighted least squares. Pure Appl. Geophys., 169(3), 467–482, doi:10.1007/s00024- 011-0381-4.

Kouichi, H. (2017). Sensors networks optimization for the characterization of atmospheric releases source, Theses, Université Paris Saclay, France. https://hal.archivesouvertes.fr/tel-01593834v2

Kouichi, H. Turbelin, G. Ngae, P. Feiz, A. A. Barbosa E. & A. Chpoun (2016), Optimization of sensor networks for the estimation of atmospheric pollutants sources, WIT Transactions on Ecology and The Environment, Vol 207, doi:10.2495/AIR160021.

Krause, A., Leskovec, J., Guestrin, C., VanBriesen, J., Faloutsos, C., (2008). Efficient Sensor Placement Optimization for Securing Large Water Distribution Networks. Journal of Water Resources Planning and Management (JWRPM).

Kumar, P., Feiz, A.-A., Ngae, P., Singh, S. K., and Issartel, J.-P.: CFD simulation of short-range plume dispersion from a point release in an urban like environment, Atmospheric Environment, 122, 645 – 656, https://doi.org/http://dx.doi.org/10.1016/j.atmosenv.2015.10.027, http://www.sciencedirect.com/science/article/pii/S1352231015304465, 2015a.

Kumar, P., Feiz, A.-A., Singh, S. K., Ngae, P., and Turbelin, G.: Reconstruction of an atmospheric tracer source in an urban-like environment, Journal of Geophysical Research: Atmospheres, 120, 12 589–12 604, https://doi.org/10.1002/2015JD024110, http://dx.doi.org/10.1002/ 2015JD024110, 2015b.

Lepley, J., Lloyd, D., Robins, A., Rudd, A., Wilks, A., 2011. Dynamic sensor deployment for the monitoring of chemical releases in urban environments (dyce). In: Chemical, Biological, Radiological, Nuclear, and Explosives (CBRNE) Sensing XII. Vol. 8018

Le, N. D., Sun, L., Zidek, J. V., (2003). Designing networks for monitoring multivariate environmental fields using data with monotone pattern. Tech. rep., Statistical and Applied Mathematical Sciences Institute, RTP, NC.

Mofarrah, A., & Husain, T. (2010). A holistic approach for optimal design of air quality monitoring network expansion in an urban area. Atmospheric Environment, 44(3), 432-440.

Ma, D., Deng, J., Zhang, Z., 2013. Comparison and improvements of optimization methods for gas emission source identification. Atmospheric Environment 81 (Supplement C), 188 - 198.

Mason, L. R., et Bohlin, J. B., (1995). Network optimization of a radionuclide monitoring system for the comprehensive nuclear test ban treaty. Tech. rep., Pacific-Sierra Research Corporation, PSR Technical Report 2585.

Saunier, O., Bocquet, M., Mathieu, A., Isnard, O., (2009). Model reduction via principal component truncation for the optimal design of atmospheric monitoring networks. Atmospheric Environment 43. 4940–4950.

Watson, J.-P., Greenberg, H. J., Hart, W. E., (2004). A multiple-objective analysis of sensor placement optimization in water networks. Proc., World Water and Environmental Resources Conf., ASCE, Reston Va.

Optimization of an Urban Urban-like Monitoring Network for Retrieving an Unknown Point Source Emission

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Abstract. This study presents a methodology for the optimization of a monitoring network of sensors measuring the polluting substances in an urban urban-like environment with a view to estimate an unknown emission source. The methodology was presented by coupling the Simulated Annealing algorithm with the renormalization inversion technique and the Computational Fluid Dynamics (CFD) modeling approach. Performance of a an obtained optimal network was analyzed by reconstructing the unknown continuous point emissions emission using the concentration measurements from the sensors in that optimized network. This approach was successfully applied and validated with 20 trials of the Mock Urban Setting Test (MUST) tracer field experiment in an urban-like environment. The optimal networks in the MUST urban region enabled are determined which makes it possible to reduce the size of original network (40-sensors) to $\sim 1/3^{rd}$ (13-sensors) and to $1/4^{th}$ (10-sensors). The 10 and 13 sensors optimal networks have estimated the averaged location errors of 19.20 m and 17.42 m, respectively, which are comparable to 14.62 m from the original 40-sensors network. In 80% trials, emission rates with the 10 and 13 sensors networks were estimated within a factor of two which are also comparable to 75% from the original network. This study presents the first an application of the renormalization data-assimilation approach for the optimal network design theory for determining the optimal monitoring networks to estimate a continuous point source emission in an urban-like environment.

1 Introduction

In case of an accidental or deliberated release of a hazardous contaminant in the densely populated urban or industrial regions, it is important to accurately retrieve the location and the intensity of that unknown emission source for the risk assessment, emergency response and mitigation strategies by the concern authority. This retrieval of an unknown source in various source reconstruction methodologies is completely dependent on the contaminant's concentrations detected by some pre-deployed sensors in that affected or a nearby region. However, pre-deployment of these limited number of sensors in that region required an optimal strategy for the establishment of an optimized monitoring network to achieve the maximum maximum a priori information regarding state of emission. It is also required to correctly capture the data while extracting and utilizing information from a limited and noisy set of the concentration measurements. The optimal monitoring networks for the characterization of the unknown emission sources in complex urban or industrial regions is a challenging problem.

The problem to optimize a monitoring network is common and consists in reducing the size of a network of sensors at the level of a city, county, or a neighborhood while retaining its properties. The positions of a small number of sensors are thus optimally determined so as to preserve the objectives of the initial monitoring network. These objectives are generally diverse, e.g., detection reconstruction of an emitting source, analysis of the air quality, triggering of an alert, etc. This study will be focused on the detection of with an objective to reconstruct an unknown continuous point source's parameters release in an urban-like environment. Using the concentration measurements from an optimally monitoring sensors network, the determination of an unknown or fabricated pollutant emissions from some industrial and accidental releases can be useful for mitigation strategies and also to impose strict actions on such pollutant sources.

This study presents a methodology for the sensor's locations choice, leading to the best network for the estimation of an unknown point point source in a geometrically complex urban environment. This type of network is of great interest in case of an accidental or intentional pollutants release because this makes it possible to estimate the sources of pollution with limited number of measurements from an optimal sensors network. In these conditions, it is necessary to know the location, and the evolution of the spatial extent of the contaminant for an emergency response. The intensity, location and time of the release are often unknown and should be inferred from sensor measurements. The source term estimation (STE) from the measurements is an inverse modeling problem. The establishment of an optimal network requires the availability of may require the sensor concentration measurements, along with the availability of meteorological data, atmospheric dispersion model, choice of a STE procedure and an optimization algorithm.

Ko et al. (1995) showed that the optimization of sensors network is an NP-hard problem(i.e. Non-deterministic Polynomial-time hardness) problem, which means that it is difficult for an exhaustive search algorithm to solve all instances of the problem because it requires a considerable time. Various optimization algorithms have been proposed to find the best solution, but these methods are not applicable to all the cases especially for large size problems. To solve such problems, the metaheuristic algorithms are efficient. Some studies discussed the optimization of sensor distribution and number for gas emission monitoring, e.g. Ma et al. (2013). Ma et al. (2013) used a direct approach with the Gaussian dispersion model to optimize the sensors networks in homogeneous terrains. However, the present study describes utilizes an inverse approach by solving the adjoint transport-diffusion equation with the building-resolving Computational Fluid Dynamics (CFD) model for an urban environment. This approach methodological approach for an optimal monitoring network (i.e. coupling of the optimization algorithm, inverse tracers transport modeling and Computational Fluid Dynamics) includes the geometric and flow complexity inherent in the an urban region for the optimization process. In this study, the Simulated Annealing (SA) stochastic optimization algorithm (Jiang et al., 2007; Abida et al., 2008; Abida and Bocquet, 2009; Saunier et al., 2009; Kouichi, 2017, etc.) (Jiang et al., 2007; Abida et al., 2008; Abida and Bocquet, 2009; Saunier et al., 2009; Kouichi et al., 2016; Kouichi, 2017, etc.) is utilized. The SA algorithm was designed for the statistical physics. It incorporates a probabilistic approach to explore the search space and converges iteratively to the solution. This algorithm is often used and recommended to solve the problems of sensors network optimization (Abida, 2010). The network optimization process consists of finding the best set of sensors that leads to the minimum of a defined cost function. A cost function can be defined as a regularized norm square of the distance between the measurements and forecasts which is also used for the STE (Sharan et al., 2012).

The STE problem for atmospheric dispersion events has been an important topic of much consideration as reviewed in Rao (2007); Hutchinson et al. (2017). Often, the source term is estimated using a network of static sensors deployed in a region. In inverse modeling process, the adjoint source-receptor relationship and concentrations and meteorological datasets are required for the STE. The adjoint source-receptor relationship is defined by an inverse computation of the atmospheric transport dispersion model (Pudykiewicz, 1998). This relationship is often affected by the nonlinearities in the flow-field by building effects in complex scenarios arising in urban environments, where the backward and forward dispersion concentrations will not match. Various inversion methods can be classified in two major categories: probabilistic and deterministic. The probabilistic category treats source parameters as the random variables associated to the probabilities probability distribution. This includes the Bayesian Estimation Theory (Bocquet, 2005; Monache et al., 2008; Yee et al., 2014, etc.), Monte Carlo algorithms using Markov chains (MCMC) (Gamerman and Lopes, 2006; Keats, 2009, etc.) and various stochastic sampling algorithms (Zhang et al., 2014, 2015, etc.). Deterministic methods use cost functions to assess the difference between observed and modeled concentrations and are based on an iterative process to minimize this difference (Seibert, 2001; Penenko et al., 2002; Issartel, 2005; Sharan et al., 2009, 2012; Kumar et al., 2015b, etc.)(Seibert, 2001; Penenko et al., 2002; Sharan et al., 2012, etc.). Among the other approaches, advanced search algorithm like genetic algorithm (Haupt et al., 2006, etc.) or neural network algorithm (Wang et al., 2015, etc.) and other regularization methods (Ma et al., 2017; Zhang et al., 2017, etc.) have been used for the STE. In this study, we focused on the renormalization inversion method (Issartel, 2005), which is deterministic in nature and does not required any initial guess for require any prior information of the source parameters. The renormalization inversion approach was successfully applied and validated for retrieval of an unknown continuous point source in flat terrain (Sharan et al., 2009, etc.) and also in urban-like environment (Kumar et al., 2015b). Initially, the renormalization inversion method was proposed to estimate emission of the distributed sources (Issartel, 2005). Sharan et al. (2009) and other studies have shown that this technique is also effective for estimating the continuous point sources. For these applications, the hypothesis of a linear relationship between the receptors receptor and the source was assumed. For homogeneous terrains, the adjoint functions can analytically be computed based on the Gaussian solution of the diffusion transport equation to estimate a continuous point release. However, the flow-field in urban or industrial environments is quite complex and the asymmetry of the flow and the dispersed plume in urban regions is generated mainly by the presence of buildings and other structures. The In general, the Gaussian models are unable to capture the effects of complex urban geometries on adjoint sensitivities between source and receptors and also if dense gases are involved, the Gaussian distribution hypothesis fails. Recently, Kumar et al. (2015b, 2016) have extended the applications of the renormalization inversion technique to retrieve an unknown emission source in the urban environments, where a CFD approach was used to generate the adjoint receptors-source relationship. In this process, a coupled CFD-renormalization source reconstruction approach was described for the identification of an unknown continuous point source located at the ground surface or at a horizontal plane corresponding to a known or predefined altitude above the ground surface, or an elevated release in an urban area.

In this study, two canonical problems are considered separately: (i) optimization of the measuring network: here, the optimization consists of selecting the best positions to be instrumented by the sensors among a set of potential locations. This choice is operated in a space of search constituted of all possible networks (of a specific size) and based on a cost function that describes quantitatively the quality of the networks. The cost function is defined from the inverse renormalization method and is quantified during the searching process. (ii) Identification of the unknown source: the STE is studied in the framework of a parametric approach using the renormalization technique. Here the challenge is to determine the parameters of the source (intensity and position) using any measurements vector (in practice the number of measurements is limited). The evoqued canonical problems are coupled in order to evaluate the performance of the proposed methodology.

The main objective of this study is to determine the sensors locations choice in an urban domain for an optimal monitoring network dedicated to estimate the location and intensity of a continuously polluting point source. A methodology was is proposed to determine an optimal network formed by a predetermined number of sensors, to better characterize a source of pollutant in a complex urban environment. This study deals with a case of reducing the number of sensors in order to obtain an optimal network from an existing network. For this purpose, a predefined network of sensors deployed in an area of interest is considered to determine an optimized network with smaller number of sensors, but, with comparable information. This work explores with two requirements of the optimal networks that modifies the spatial configuration of an existing network by moving the sensors and also reduces the number of sensors of an existing large network. In real situation this methodology can be applied for the optimization of mobile networks deployed in emergency situation. The methodological approach to optimize the monitoring network in urban environment was presented by coupling the SA stochastic algorithm with the renormalization inversion technique and the CFD modeling approach. The concentration measurements from these optimized networks of sensors in 20 trials of the Mock Urban Setting Test (MUST) field tracer experiment were utilize to validate the methodology to retrieve an unknown continuous point source in an urban-like environment.

2 Source Term Estimation Method: The Renormalization

In the context of an inversion approach, source parameters are often determined using the concentrations concentration measurements at the sensor locations and a source-receptors relationship. The release is considered continuous from a point source located at the ground or at an a horizontal plane corresponds to an altitude of a known source height. The renormalization inversion Since the optimization methodology presented in the next section utilizes some concepts from the renormalization inversion methodology (Sharan et al., 2009), the renormalization theory to estimate a continuous point release is briefly presented in following subsections.

2.1 Source-Receptor relationship

The A source-receptor relationship is an important concept in the source reconstruction process and it can be linear or nonlinear. This study deals with the linear relationship, as except from the nonlinear chemical reactions, most of the other processes occurring during the atmospheric transport of trace substances are linear: advection, diffusion, convective mixing, dry and wet deposition, and radioactive decay (Seibert and Frank, 2004). A source-receptor relationship between the measurements and the source function is defined based on a solution of the adjoint transport-diffusion equation that exploits the computed adjoint functions (retroplumes) corresponding to each receptor (Pudykiewicz, 1998; Issartel et al., 2007, etc.). These retroplumes provide a sensitivity information between the source position and the sensor locations. Let's consider a discretized domain of N grid cells in a 2-dimensional space $\mathbf{x} = (x, y)$, a vector of M concentration measurements $\boldsymbol{\mu} = (\mu_1, \mu_2, ..., \mu_M)^T \in \mathbb{R}^M$, and an unknown source vector $\mathbf{s}(\mathbf{x}) \in \mathbb{R}^N$ to estimate. The measurements $\boldsymbol{\mu}$ are related to the source vector $\mathbf{s}$ by the use of sensitivity coefficients (also referred as adjoint functions) (Hourdin and Talagrand, 2006). The sensitivity coefficients describe the backward propagation of information from the receptors toward the unknown source. These vectors are related by the following linear relationship:

$$\boldsymbol{\mu} = \mathbf{A}\mathbf{s} + \boldsymbol{\epsilon} \tag{1}$$

where $\boldsymbol{\epsilon} \in \mathbb{R}^M$ is the total measurements error and $\mathbf{A} \in \mathbb{R}^{M \times N}$ is the sensitivity matrix with $\mathbf{A}(\mathbf{x}) = [\mathbf{a}(\mathbf{x}_1), \mathbf{a}(\mathbf{x}_2), ..., \mathbf{a}(\mathbf{x}_N)]$. Here, each column vector $\mathbf{a}(\mathbf{x}_i) \in \mathbb{R}^M$ of the matrix $\mathbf{A}$ represents the potential sensitivity of a grid cell with respect to all M concentration measurements.

For a given set of the concentration measurements $\boldsymbol{\mu}$, the source estimate function $\mathbf{s}(\mathbf{x})$ in Eq. (1) can easily be estimated by formulating a constrained optimization problem. This optimization problem minimizes a cost function $J(\mathbf{s}) = \mathbf{s}^T\mathbf{s}$, subjected to a constraint $\boldsymbol{\epsilon} = \boldsymbol{\mu} - \mathbf{A}\mathbf{s} = 0$. Using the method of Lagrange multipliers, $\mathbf{s}(\mathbf{x})$ can be estimated as a least-norm solution(Kumar et al., 2016):

$$\mathbf{s} = \mathbf{A}^T\mathbf{H}^{-1}\boldsymbol{\mu} \tag{2}$$

where $\mathbf{H}^{-1}$ is inverse of the *Gram matrix* $\mathbf{H} = \mathbf{A}\mathbf{A}^T$. This estimate (Eq. (2)) is not satisfactory because it generates artifacts at the grid cells corresponding to the measurement points. Adjoint functions become singular at these points and have very large values. These large values do not represent a physical reality, but rather an artificial information. This was also highlighted by Issartel et al. (2007) which reduced this artificial information by a process of renormalization.

2.2 Renormalization process

This process involves a weight function in space $\mathbf{W}(\mathbf{x}) \in \mathbb{R}^{N \times N}$, which is purely a diagonal matrix with the diagonal elements $w_{jj} > 0$ such that $\sum_{i=1}^{N} w_{jj} = M$. Introduction of $\mathbf{W}$ transforms the source-receptor relationship in Eq. (1) to:

$$\boldsymbol{\mu} = \mathbf{A}_w\mathbf{W}\mathbf{s} + \boldsymbol{\epsilon}. \tag{3}$$

where the modified sensitivity matrix $\mathbf{A}_w$ is defined as $\mathbf{A}_w = \mathbf{A}\mathbf{W}^{-1} = [\mathbf{a}_w(\mathbf{x}_1), \mathbf{a}_w(\mathbf{x}_2), ..., \mathbf{a}_w(\mathbf{x}_N)]$ in which the column vector $\mathbf{a}_w(\mathbf{x}_i) = \mathbf{a}(\mathbf{x}_i)/w(\mathbf{x}_i)$ of $\mathbf{A}_w$ is the weighted sensitivity vector at $\mathbf{x}_i$. Considering a similar approach that outlined in previous subsection, a new constrained optimization problem can be formulated for Eq. (3) to estimate $\mathbf{s}(\mathbf{x})$. This optimization problem minimizes a cost function $J(\mathbf{s}) = \mathbf{s}^T\mathbf{W}\mathbf{s}$, subjected to a constraint $\boldsymbol{\epsilon} = \boldsymbol{\mu} - \mathbf{A}_w\mathbf{W}\mathbf{s} = 0$, and deduces the following expression $\mathbf{s}_w$ of $\mathbf{s}$ (Kumar et al., 2016)(Appendix A in Kumar et al., 2016):

$$\mathbf{s}_w = \mathbf{A}_w^T\mathbf{H}_w^{-1}\boldsymbol{\mu} \tag{4}$$

where $\mathbf{H}_w^{-1}$ is the inverse of $\mathbf{H}_w = \mathbf{A}_w\mathbf{W}\mathbf{A}_w^T$.

2.3 Weight function

Issartel et al. (2007) demonstrated that a weight function , which reduces the artifacts of the adjoint functions at the measurement points, must verify the following renormalization criterion:

$$\mathbf{a}_w^T(\mathbf{x})\mathbf{H}_w^{-1}\mathbf{a}_w(\mathbf{x}) \equiv 1$$

Following The weight function in the above discussed renormalization process is computed by using an iterative algorithm by Issartel et al. (2007), $w(\mathbf{x})$is determined as: demonstrated by Issartel et al. (2007) (Appendix A).

$$w_0(\mathbf{x}) = 1, \quad \text{and} \quad w_{k+1}(\mathbf{x}) = w_k(\mathbf{x})\sqrt{\mathbf{a}_{wk}^T(\mathbf{x})\mathbf{H}_{wk}^{-1}\mathbf{a}_{wk}(\mathbf{x})}$$

2.3 Identification of point source

Consider a point source of continuous release at a position $\mathbf{x_o} = (x_o, y_o)$ and with the intensity q_o. The point source is thus expressed as a function of the preceding parameters: $\mathbf{s}(\mathbf{x}) = q_o\delta(\mathbf{x} - \mathbf{x_o})$. The relationship between the source and the measurements (Eq. (3)) becomes: $\boldsymbol{\mu} = q_o\mathbf{a}_w(\mathbf{x_o})w(\mathbf{x_o}) + \boldsymbol{\epsilon}$. By replacing the measurement term in Eq. (4), one obtains:

$$\mathbf{s}_w = q_o w(\mathbf{x_o})\mathbf{A}_w^T\mathbf{H}_w^{-1}\mathbf{a}_w(\mathbf{x_o}). \tag{5}$$

$\mathbf{s}_w$ reaches its maximum at position $\mathbf{x_o}$ as the renormalization criterion (Eq. (A1)) is satisfied only at this position $\mathbf{x_o}$. Thus, $\mathbf{s}_w(\mathbf{x})$ at $\mathbf{x_o}$ becomes:

$$\mathbf{s}_w(\mathbf{x_o}) = q_o w(\mathbf{x_o}), \tag{6}$$

which estimates the source intensity $q_o = \mathbf{s}_w(\mathbf{x_o})/w(\mathbf{x_o})$.

3 The Combinatorial Optimization of a Monitoring Network

A predefined large network of n sensors deployed in an area of interest is considered to determine an optimized network with smaller number of sensors, but with comparable information. For a given number of p sensors such that $p < n$, one determines an array of p sensors among n, which delivers maximum of the information. It is a combinatorial optimization problem that consists of choosing p sensors among n, and thus constituting an optimal network. The optimal network will consist of p sensors for which a defined cost function is minimum. The number of possible choices ${}^nC_p$ (number of combinations of p among n) is very high, when an initial network is sufficiently instrumented (n large) and p is small with respect to n. As the number of combinations to be tested is very large, minimum of a cost function will be evaluated by a stochastic algorithm, viz. simulated annealing (SA).

3.1 Cost function

A cost function is defined (based on the renormalization theory) as a function that minimizes the quadratic distance between the observed and the simulated measurements according to the $\mathbf{H}_w$ norm (Issartel et al., 2012). $\mathbf{H}_w$ is the *Gram matrix* defined in a previous section 2.2. As the cost function is convex, its minimum value must also correspond to the maximum intensity of the source. The quadratic distance between the real and the simulated concentration measurements according to the $\mathbf{H}_w$ norm is given by :

$$J_s = \|\boldsymbol{\mu} - \hat{\boldsymbol{\mu}}\|^2_{\mathbf{H}_w^{-1}} = \frac{1}{2}\left[(\boldsymbol{\mu} - \hat{\boldsymbol{\mu}})^T \mathbf{H}_w^{-1} (\boldsymbol{\mu} - \hat{\boldsymbol{\mu}})\right] \tag{7}$$

When considering a point source, $\hat{\boldsymbol{\mu}}$ is written by $\hat{\boldsymbol{\mu}} = q\mathbf{a}_w(\mathbf{x})w(\mathbf{x})$, where q and $\mathbf{x}$ $\hat{\boldsymbol{\mu}} = q_o\mathbf{a}_w(\mathbf{x})w(\mathbf{x})$, where q_o and $\mathbf{x}$ are respectively the intensity and the position vector of a of a point source. By replacing $\hat{\boldsymbol{\mu}}$ in Eq. (7), one obtains (Sharan et al., 2012; Issartel et al., 2012):

$$J_s = J_s(q_o, \mathbf{x}) = \frac{1}{2}\left[(\boldsymbol{\mu} - q_o\mathbf{a}_w(\mathbf{x})w(\mathbf{x}))^T H \mathbf{H}_w^{-1}(\boldsymbol{\mu} - q_o\mathbf{a}_w(\mathbf{x})w(\mathbf{x}))\right] \tag{8}$$

The conditions of maximum intensity and convexity are expressed by two following equationsFor a fixed $\mathbf{x}$ in Eq. (8), J reaches a strict local minimum if following two conditions are satisfied:

$$\frac{\partial J_s(q,\mathbf{x})}{\partial q} \frac{\partial \mathrm{J}(\mathrm{q_o},\mathbf{x})}{\partial \mathrm{q_o}} = 0 \tag{9}$$

$$\frac{\partial^2 J_s(q,\mathbf{x})}{\partial q^2} \frac{\partial^2 \mathrm{J}(\mathrm{q_o},\mathbf{x})}{\partial \mathrm{q_o^2}} > 0 \tag{10}$$

For each fixed $\mathbf{x}$, the first condition (Eq. (9)) gives an estimate ($\tilde{q_0}$) of q_0 as: $\tilde{q_0} = \frac{\mathbf{a}_w^T(\mathbf{x})\mathbf{H}_w^{-1}\boldsymbol{\mu}}{w(\mathbf{x})}$. The second condition (Eq. (10)) is always satisfied as $\frac{\partial^2 J(q,\mathbf{x})}{\partial q^2} = w^2(\mathbf{x}) > 0, \forall \mathbf{x}$ (Sharan et al., 2012). Sharan et al. (2012) has also shown that $\frac{\partial^2 J(q_o,\mathbf{x})}{\partial q_o^2} = w^2(\mathbf{x}) > 0, \forall \mathbf{x}$ (Sharan et al., 2012). Corresponding to the estimate $\tilde{q_0}$ from the first condition (Eq. (9))leads to following expression of J_s, the cost function J from Eq. (8) leads to the following expression (Issartel et al., 2012):

$$J_s(\tilde{q_0},\mathbf{x}) = \frac{1}{2}\frac{\boldsymbol{\mu}^\mathrm{T}\mathbf{H}_\mathrm{w}^{-1}\boldsymbol{\mu}}{2}\left[1 - \frac{\mathbf{s}_w^2}{\boldsymbol{\mu}^T\mathbf{H}_w^{-1}\boldsymbol{\mu}}\right] \tag{11}$$

where $\mathbf{s}_w$ is same as given in Eq. (4) and $\boldsymbol{\mu}^T\mathbf{H}_w^{-1}\boldsymbol{\mu}$ is a positive constant. Considering Eq. , it appears (11), it is obvious that the minimization of $J_s(\mathbf{x})$ J also corresponds to the maximization of the term $\frac{\mathbf{s}_w^2}{\boldsymbol{\mu}^T\mathbf{H}_w^{-1}\boldsymbol{\mu}}$. or minimization of term $\left[1 - \frac{\mathbf{s}_w^2}{\boldsymbol{\mu}^T\mathbf{H}_w^{-1}\boldsymbol{\mu}}\right]$. Accordingly, the minimum value of the cost function J in Eq (11) leads to the following expression of the cost function (say $J_s(\mathbf{x})$) to minimize:

$$\mathrm{J_s}(\mathbf{x}) = 1 - \frac{\mathbf{s}_\mathrm{w}^2}{\boldsymbol{\mu}^\mathrm{T}\mathbf{H}_\mathrm{w}^{-1}\boldsymbol{\mu}} \tag{12}$$

A global minimum of the cost function $J_s(\mathbf{x})$ is evaluated by the SA algorithm.

3.2 Simulated Annealing (SA) algorithm for the Sensor's Network Optimization

The SA algorithm is problem of optimization of a network is solved using the simulated annealing (SA) algorithm. The SA optimization algorithm is utilized here for the determination of the optimal networks by comparing its performance with the Genetic Algorithm (GA)(Kouichi, 2017). These algorithms of different search technics (SA probabilistic and GA evolutionary) are evaluated based on the same cost function. The results showed that the optimal networks retained by the GA and the SA are quantitatively and qualitatively comparable (Kouichi, 2017). The SA has advantageous because it is relatively easy to implement and takes smaller computational time in comparison to GA. Both SA and GA optimization algorithms in the framework of this approach (based in the renormalization theory) has little influence on the estimation of the parameters of a source (Kouichi, 2017).

The SA is a random optimization technique based on an analogy with thermodynamics. To find a global minimum, it incorporates the temperature The technique has been introduced to the computational physics over sixty years ago in the classic paper by Metropolis et al. (1953). The algorithm of simulated annealing is initiated by starting from an admissible network. At the subsequent steps, the system moves to another feasible network, according to a prescribed probability, or it remains in the current state. However, it is crucial to explain how this probability is calculated. The mobility of the random walk depends on a global parameter T which is interpreted as 'temperature'. The initial values of T are large, allowing free exploration of large extents of the state space (this corresponds to the "melted state" in terms of the kinetic theory of matter). In the subsequent steps, the temperature is lowered allowing the algorithm to reach a local minimum.

For the SA, each network is considered as a state of a virtual physical system, and the objective function is interpreted as the internal energy of this system in a given state. According to statistical thermodynamics, the probability of a physical system for being in a same state follows the Boltzmann distribution and depends on its internal energy and the temperature level. By analogy, the physical quantities (temperature, energy, etc.) become a pseudo-quantities. And during the minimization process, the probabilistic treatment consists to accept a new network selected in the neighborhood of the current network following the same Boltzmann distribution and depending both on the cost difference between the new and the current networks and on the pseudo-temperature ('temperature'). To find the solution, the SA incorporates the 'temperature' into a minimization procedure. So at high temperature (starting temperature'temperature' (starting 'temperature'), the space of solution is widely explored, while at lower temperature 'temperature' the exploration is restricted. The algorithm is stopped when the cold temperature 'temperature' is reached. It is necessary to choose the law of decreasing temperature'temperature', called as cooling schedule. Different approaches to parameterize the SA are explored in Siarry (2016). Kirkpatrick et al. (1983) proposed an average probability to determine the initial (starting) temperature'temperature'. Nourani and Andresen (1998) compared the most used cooling schedules (exponential, logarithmic, and linear). The SA algorithm starts minimization of an objective function at annealing temperature 'temperature' from a single stochastic point, then it searches for the minimal solutions by attempting all the points in search domain with respect to their value of the temperature'temperature'. The algorithm is depicted in a flow diagram in Figure 2 and a step by step implementation of the SA procedure for an optimized monitoring network in an urban environment is described as follows:

Step 1. Parameters setting and initialization

Network parameters (n and p): n is the number of possible locations of the sensors and p is the optimal network number of sensors.

Starting 'temperature' (T_0): T_0 is also called the highest temperature'temperature'. It was determined from the Metropolis law: $T_0 = -\frac{\overline{(\Delta J_s)}}{log(P_0)}$, where $\overline{(\Delta J_s)}$ is an average of the difference of cost functions calculated for a large number of cases. P_0 is an acceptance probability and following the recommendations of Kirkpatrick et al. (1983), it was set to 0.8. Start iterations ($I_{tt} = 0$).

Length of the bearing (L_{max}): A length of the bearing is the number of iterations to be performed at each temperature 'temperature' level. An equilibrium is reached for this number of iterations and any significant improvement of the cost function can be expected. No general rule is proposed to determine a suitable length. This number is often constant and proportional to the size of the problem.

The 'temperature' decay factor (θ): The temperature 'temperature' remains constant for L_{max} iterations corresponding to each bearing. We used the exponential schedule due to its efficiency as denoted by Nourani and Andresen (1998). Then, the temperature 'temperature' decreases law between two bearings varies as: $T_{b+1} = \theta T_b$, with $0 < \theta < 1$, where b represents a bearing. So, it was retained a decay pattern by the bearings.

The cold 'temperature' (T_{cold}): T_{cold} is often called the stopping temperature'temperature'. There is no clear rule to set this parameter. It is possible to stop calculations when no improvement in the cost function is observed during a large number of combinations. One can estimate this number and take into account the maximum length L_{max} of each bearing, thus the cold temperature 'temperature' can be expressed as a fraction of the starting temperature 'temperature' T_0.

Assigning the first best set of sensors, $\mathbf{x}_{Best} \leftarrow \mathbf{x}_{rand}(p,n)$: $\mathbf{x}_{rand}(p,n)$ corresponds to a vector of p sensors locations randomly chosen among the *n* possible locations. A new solution is randomly explored. This vector is assigned to the first 'best' set of sensors.

Step 2. Assigning a new set of sensors

$\mathbf{x}_{new} \leftarrow \mathbf{x}_{rand}(p,n)$, where $\mathbf{x}_{rand}(p,n)$ corresponds to a vector of p sensors locations randomly chosen among the *n* possible locations. This vector is assigned to a new set ($\mathbf{x}_{new}$) of the sensors.

Step 3. Cost difference

Given a sensor location $\mathbf{x}_{new}$, the cost function $J_s(\mathbf{x}_{new})$ is computed as follows:

- set $\boldsymbol{\mu}$ vector by using the measurements at the $\mathbf{x}_{new}$ locations,
- set rows of matrix $\mathbf{A}$ using the sensitivity at the $\mathbf{x}_{new}$ locations,
- determine $w(\mathbf{x})$, $\mathbf{H}_w$, and $\mathbf{a}_w$ iteratively using the algorithm in Eq. (A2),
- compute the source term $\mathbf{s}_w(\mathbf{x})$ using Eq. (4),

- compute the cost function $J_s(\mathbf{x}_{new})$ using Eq. (12).

$J_s(\mathbf{x}_{best})$ is computed like $J_s(\mathbf{x}_{new})$ using the same precedent steps. A cost difference is then calculated using $\Delta J_s = J_s(\mathbf{x}_{new}) - J_s(\mathbf{x}_{best})$. Increment the iterations $(I_{tt} \leftarrow I_{tt} + 1)$.

Step 4. Test of sign of ΔJ_s

If $\Delta J_s < 0$, the error associated with $\mathbf{x}_{new}$ is less than that with $\mathbf{x}_{best}$ and thus $\mathbf{x}_{new}$ will become the next 'best network' (*Step* 6). If this condition is not satisfied, the algorithm can jump out of a local minimum (*Step* 5).

Step 5. Conditional jump

When $\Delta J_s > 0$, the algorithm has ability to jump out any local minima if condition: $P_{01} \leq \exp(-\frac{\Delta J_s}{T})$ is satisfied, where P_{01} is the acceptance probability (a random number between 0 and 1), and T is the current annealing temperature'temperature'. It means that $\mathbf{x}_{new}$ will be the next 'best network' even if the associated error is greater than that of $\mathbf{x}_{best}$. If $P_{01} > \exp(-\frac{\Delta J_s}{T})$, go to *Step* 7.

Step 6. Update $\mathbf{x}_{best}$

In this step, $\mathbf{x}_{best}$ is updated by $\mathbf{x}_{new}$.

Step 7. Maximum iteration check

If the maximum number of iterations of a bearing (L_{max}) is reached, a state of equilibrium is then achieved for this temperature 'temperature' and one can cool the actual temperature 'temperature' (*Step* 8). If not, continue iterations (*Step* 2).

Step 8. 'Temperature' cooling

Temperature 'Temperature' is cooled using the cooling schedule and iteration variable is reset to zero.

Step 9. Cold 'temperature' test

The cold temperature 'temperature' (T_{cold}) is also known as the stopping temperature'temperature'. If this temperature 'temperature' is reached, the algorithm is stopped. When T_{cold} is not reached, other temperature 'temperature' bearing are performed using the cooling schedule.

Step 10. Optimal network

At this step, the last best network $\mathbf{x}_{best}$ is the optimal network. Source parameters are then estimated using the concentration measurements and retroplumes only for sensors from the obtained optimal network as: (i) $\mathbf{x}_0$ is estimated at position of the maximum of the source estimate function $\mathbf{s}_w(\mathbf{x})$, and (ii) the intensity q_0 is given by $q_0 = \mathbf{s}_w(\mathbf{x}_0)/w(\mathbf{x}_0)$.

In stochastic optimization algorithms, especially in the SA, it was observed that there is no guarantee for the convergence of the algorithm with such a strong cooling (Cohn and Fielding, 1999; Abida et al., 2008). However, chances are that a near-optimal network configuration can be reached. Due to this, one or more near-optimal networks can be obtained from this methodology that satisfy the conditions of near overall optimum condition.

4 The Mock Urban Setting Test (MUST) Tracer Field Network

The MUST field experiment was conducted by the Defense Threat Reduction Agency (DTRA) in 2001. It was aimed to help developing and validating the numerical models for flow and dispersion in an idealized urban environment. The experimental design and observations are described in detail in Biltoft (2001) and Yee and Biltoft (2004). In this experiment, an urban canopy was represented by a grid of 120 containers. These containers were arranged along 12 rows and 10 columns on the army ground in the Utah desert, USA. Each container has dimensions of 2.54 m high, 12.2 m long and 2.42 m wide. The spacing between the horizontal lines is 12.9 m, while the columns are separated by a distance of 7.9 m. The total area thus formed is approximately 200×200 m^2. The experiment consists of 63 releases of a flammable gas (propylene C_3H_6) that is not dangerous or harmful in quantities and could be released through the dissemination system into the open atmosphere (Biltoft, 2001). Different wind conditions (direction, speed, atmospheric stability) as well as different positions for gas emissions (inside or outside the MUST urban canopy at different heights) were considered. These gas emissions were carried out under stable, very stable, and neutral stability conditions. In this study, 20 trials in various atmospheric stability conditions are selected and the meteorological variables are taken from an analysis of meteorological and micro-meteorological observations in Yee and Biltoft (2004) (Table 1). It is noted that the errors related to meteorological data can affects the accuracy of the source term estimation (Zhang et al., 2014, 2015), although this error is not considered in this study. In each trial, the gas was continuously released for ≈ 15 min, during which the concentration measurements were made. These concentration measurements were carried out by 48 photoionization detectors (PIDs). 40 sensors were positioned on four horizontal lines at 1.6 m height (Figure 1) and 8 sensors were deployed in vertical direction at a tower located approximately in center of the MUST array.

5 CFD Modelling for Retroplumes in an Urban Environment

The flow-field in atmospheric dispersion models in geometrically complex urban or industrial environments cannot be considered as homogeneous throughout the computational domain. This is because the buildings and other structures in that region influence and divert the flow into unexpected directions. Consequently, the dispersion of a pollutant and computations of the adjoint functions (retroplumes) are affected by the flow-field induced by these structures in an urban region. Recently, Kumar et al. (2015b) Kumar et al. (2015a) utilized a CFD model to compute the flow-field and then the forward dispersion in 20 trials of the MUST field experiment. In order to reconstruct an unknown continuous point source, the computed flow-field is then used to compute the retroplumes for all selected trials in the MUST experiment(Kumar et al., 2015b). A CFD model fluidyn-PANACHE was utilized to calculate the flow-field, considering a subdomain of calculation (whose dimensions are 250×225 m^2 with a height of 100 m) that consists the MUST urban array created by the containers, sources, receptors, and other instruments in this experiment. This subdomain is embedded in a larger computational domain (dimensions of 800 $\times$ 800 m^2 with a height of 200 m) to ensure a smooth transition of the flow between the edges of the domain and the obstacles zone. This extension of the outer domain far from the main experimental site is essential to reduce effects of the inflow boundary conditions imposed at inlet of the outer domain. A more detailed description about the CFD model and its simulations for the MUST field experiment, e.g., boundary conditions, turbulence model, etc. is briefly presented in are presented in Kumar et al. (2015a) and now briefly discussed in the Supplementary Information (SI). An unstructured mesh was generated in both domains with more refinement in the urbanized area in inner subdomain and at the positions of receptors, thus generating 2849276 meshes.

The simulations results with fluidyn-PANACHE in each MUST trial were obtained with inflow boundary conditions from vertical profiles of the wind (U), the turbulent kinetic energy (k) and its dissipation rate (ϵ). These inflow profiles include: *(i) Wind profile*: Gryning et al. (2007) profiles in stable and neutral conditions and a profile based on the stability function by Beljaars and Holtslag (1991) in very stable conditions, *(ii) Temperature profile:* Monin-Obukhov similarity theory based logarithmic profiles, *(iii) Turbulence profiles:* k and ϵ profiles are based on an approximate analytical solution of one-dimensional $k-\epsilon$ prognostic equations (Yang et al., 2009). The atmospheric stability effects in the CFD model fluidyn-PANACHE are included through the inflow boundary condition (via advection). fluidyn-PANACHE includes a Planetary Boundary Layer (PBL) model that serves as an interface between the meteorological observations and the boundary conditions required by the CFD solver. The observed turbulence parameters, e.g. (i) sensible heat flux (Q_h), the Obukhov length (L), (iii) surface friction velocity (u_*) and the temperature scale (θ_*) were used to derive the vertical profiles of mean velocity and potential temperature. As an example, the wind velocity vectors around some containers for the trial 11 are shown in SI Figure S1.1. This figure shows the deviations in the wind speed and its direction due to the obstacles in an urban-like environment. It should be noted that the MUST experiment took place under neutral to stable and strongly stable conditions. However, the only atmospheric stability effects included in the CFD model are through the specification of inflow boundary conditions. Atmospheric stability has a profound impact on dispersion and would thus influences the adjoint functions. However, as presented and discussed in our previous study (Kumar et al., 2015a), even with specification of the stability dependent inflow boundary conditions only, the predicting forward concentrations from the CFD model are in good agreement with the measured concentrations for all 20 trials in different atmospheric stability conditions. However, at micro-scales also, small irregularities can break the repeated flow patterns found in a regular array of containers with identical shape (Qu et al., 2011). In addition, uncertainties associated with the thickness and the properties of the material of the container wall also affect flow pattern and the resulted concentrations and adjoint functions (Qu et al., 2011). Accordingly, the atmospheric stratification and stability effects should also be included through surface cooling or heating in the CFD model and stability effects from inflow boundary conditions. Since the released gas propylene is heavier than the air and would behave as a dense gas, a buoyancy model was used to model the body force term in the Navier-Stokes equations. The buoyancy model is suitable for the dispersion of heavy gases where density difference in the vertical direction drives the body force.

In order to compute the retroplumes in each MUST trial, firstly the CFD simulations were performed to compute the converged flow-field in computational domain, secondly the flow-field is reversed and used in the standard advection-diffusion equation to compute the adjoint functions $\mathbf{a}_i(\mathbf{x})$. In this computation of the retroplumes corresponding to each receptor in a selected trial, the advection-diffusion equation is solved by considering a receptor as a virtual point source with unit release rate at the height of that receptor. Also, the meteorological conditions remained invariant during the whole experimental period in a trial. The details about the retroplumes and the correlated theory of the duality verification (i.e. comparison of the concentrations predicted with the forward (direct) model and the adjoint model) for all 20 trials of the MUST field experiment are given in Kumar et al. (2015a)Kumar et al. (2015b). Since we are concerned to establish an optimized monitoring network in a domain that contains the MUST urban array, the retroplumes are computed in the inner subdomain only. Consequently all the computations for an optimized monitoring network were carried out in the inner subdomain only. The sensors in the optimized monitoring network are supposed to deploy on a fixed vertical height above the ground surface. Accordingly, the retroplumes corresponding to only 40 receptors at 1.6 m height were utilized in computations for the optimized monitoring networks in the MUST urban environment.

6 Results and Discussion

The calculations were performed by coupling the SA algorithm to a deterministic renormalization inversion algorithm and the CFD adjoint fields to optimize the monitoring network in an urban urban-like environment of the MUST field experiment. The network optimization process consists of finding the best set of sensors that leads to the lowest cost function. In this study, the validation is realized following two separated steps. The first step consists to form two optimal monitoring networks were formed to have the sizes reduced by by using the presented optimization methodology which makes it possible to reduce the size of original network of 40 sensors to approx. one-third (~ 13 13 sensors) and one-fourth (10 sensors)respectively compared to the initial network. The second step consists to compare a posteriori the performance of the obtained optimal networks to the 'MUST predefined network' of 40 sensors at 1.6 m above the ground surface. In first step, the comparison with networks of the same size (e.g. 10 sensors) was performed implicitly during the optimization process. As the SA is an iterative algorithm, during the optimization process networks of same size are compared at each iteration and the 'best one' is retained. The networks have also been generated randomly like in Efthimiou et al. (2017); however, the search space of the problem is very large. In our case, the number of the compared networks is equivalent to the number of iterations (as an example for optimal network of 10 sensors $\sim 3 \times 10^4$ configurations are compared). Here, the comparison is based on a cost function and inspired from the renormalized data assimilation method. The cost function quantifies the quadratic distance between the observed and the simulated measurements. The 'optimal network' produces the 'best' description of the observations (i.e. corresponds to the minimal quadratic distance) and permits a posteriori to estimate the location and emission rate of an unknown continuous point source in an urban-like environment.

The size of the 'MUST predefined (original) network' is 40 sensors and the sizes of the optimized networks are fixed after performing a first optimization with the number of sensors from 4 to 16 (Kouichi, 2017). This first evaluation showed that for some trials, a small number of sensors could not allow to correctly reconstruct the source and divergences in the calculations have been noted. Accordingly, the source estimation obtained for different trials and network sizes show that, very often, networks of less than 8 sensors can not correctly characterize the source. On the other hand, beyond 13 sensors, the source estimation is not significantly improved, and the associated errors were roughly constant (Kouichi, 2017). Therefore, in order to ensure an acceptable estimate of the source for all the trials, the sizes of the optimized network are fixed as 10 and 13 sensors ($1/4^{th}$ and $\sim 1/3^{rd}$ respectively of the original network of 40 sensors).

The optimization calculations were performed using Matlab on a computer with configuration "Intel® Core™ i7-4790 CPU @ 3.60 GHz and 16 GB RAM". The averaged computational time for optimization of one 10 sensors network was ≈ 2.5 hrs and ≈ 8.5 hrs for 13 sensors network. In computations, a value of parameter $T_0 = 10$ was fixed according to the scale of cost function and using the methodology described in *Step* 1 and $T_{cold} = 10^{-13}$ was used for both the optimal sensors networks. θ is a decay factor of the temperature 'temperature' for an exponential cooling schedule that describes a procedure of the temperature decrease. The best cooling schedule is the exponential decay as demonstrated by Nourani and Andresen (1998); Cohn and Fielding (1999). θ was fixed as 0.9 following the recommendation in literature (Siarry, 2014). This value allows a sufficiently slow cooling in order to give more chance to the algorithm to explore a large search space and to avoid the local minima. L_{max} is taken as 100 & 200 for 10 & 13 sensors networks, respectively, following the recommendation in Siarry (2014) and according to number of the possible combinations that increases with the number of sensors (8.5×10^8 for 10 sensors and 1.2×10^{10} for 13 sensors).

Figure 3 shows the optimal networks of 10 and 13 sensors respectively for three representative trials 5 (very stable), 11 (neutral), and 19 (stable) in the MUST urban array. These three trials correspond to one trial each in neutral, stable, and very stable atmospheric conditions during the release. The optimal monitoring networks of 10 and 13 sensors for all selected 20 MUST trials are shown in SI Figures S1S2.1&S1S2.2.

In order to analyze the performance of the optimal monitoring configurations, the source reconstructions were performed to estimate the unknown location and the intensity of a continuous point release. These source reconstruction results were obtained from the optimal monitoring networks formed by 10 and 13 sensors in each MUST trial. In this, the retroplumes and the concentration measurements were utilized from the sensors corresponding to these optimal networks. The retroplumes were computed using CFD simulations, considering the dispersion in a complex terrain. The source reconstruction results from both the optimal monitoring networks were also compared with results computed from the initial MUST network formed by 40 sensors (Kumar et al., 2015b). As in practice, the number of measurements is limited, this comparison allowed concluding that in urban areas, the reduction of networks size is possible and does not degrade significantly its efficiency in source estimation.

Source estimation results from the different monitoring networks are shown in Table 2 for all 20 selected trials of the MUST experiment. These results are presented in terms of the location error (E_l^p), which is an euclidean distance between the estimated and the true source location, and E_q^p, a ratio of the estimated to the true source intensity. The corresponding monitoring network is represented by a superscript p (representing the number of sensors in a an optimal network) on E_l^p and E_q^p. In order to quantify the uncertainty, a 10% Gaussian noise was added at each measurements. Accordingly, 50 simulations for the source reconstruction were performed with these noise measurements using the optimal networks for each trial. The average and the standard deviation of E_l^p and E_q^p are calculated and the result are also presented in Table 2.

For a given trial, a parameter *skeleton* represents the common sensors between two optimal networks of different sizes (with 10 and 13 sensors). These results exhibit that the SA algorithm coupled with renormalization inversion theory and CFD modeling approach has succeeded in proposing the good optimal monitoring networks to estimate the unknown emissions in an urban environment.

Figure 4 shows isopleths of the renormalized weight function (also called as the visibility function) and the normalized source estimate function $\mathbf{s}_w^n(\mathbf{x}) = \mathbf{s}_w(\mathbf{x})/\max(\mathbf{s}_w(\mathbf{x}))$ correspond to both optimal monitoring networks for three representative trials (e.g. 5, 11, and 19) of the MUST experiment. These isopleths for all selected 20 MUST trials are shown in SI Figures S2S3. A statistical parameter, factor of g (FAg), for the source reconstruction results from each monitoring network is presented in Table 3, where FAg represents the percentage no. of trials in which the source intensity is estimated within a factor of g. The statistics calculated with 40 sensors network show that the average location error for all 20 trials is 14.62 m, and in 75% of the trials, the intensity of the source is estimated within a factor of two. In 90% of the trials, intensity was estimated within a factor of three and within a factor of four in 95% trials (Table 3). If trial 2 is considered, large location errors (greater than 30 m) and the intensity values ranged between a factor of three to five, were observed (Table 2) independently of the number of sensors in the networks (Table 2). If we consider the trials 15, 16, & 20, it was noted that the larger location errors do not necessarily correspond to the high intensity errors (Table 2).

From distribution of the optimized sensors in networks in Figures 3 for trials 5, 11 & 19 and SI Figures S1S2.1&S1S2.2 for all selected trials, it was noted that a larger number of sensors are close to the source position in the optimal networks in most of the trials. This tendency makes it possible for sensors from an optimal network to monitor the region where a source can be located and it can be explained in terms of the visibility function. The visibility function includes the natural information associated with a monitoring network for the source retrieval in a domain and physically interprets the extent of regions seen by the network (Issartel, 2005; Sharan et al., 2009). The visibility function is independent of the effective values of the concentration measurements and depends only on geometry of the monitoring network. Hence, this leads to a priori information about the unknown source apparent to the monitoring network. It was observed that the visibility functions have significant levels at the source positions (Figures 4 & S2S3).

The source reconstruction results from the optimal monitoring networks formed by 10 sensors have an averaged location error (E_l^{10}) of 19.20 m for all 20 trials in the MUST experiment (Tables 2&3). In most of the trials, the location and the intensity of a continuous point emission are estimated accurately and close to the true source parameters. The location error is minimum in trial 14 (E_l^{10} = 5.50 m) and maximum in trial 2 (E_l^{10} = 56.88 m) (Table 2). For this configuration of the optimal sensors network, the source intensity in 80% of the trials are estimated within a factor of two to their true release rates (Tables 2&3).

For all 20 trials, the averaged location error E_l^{13} is 17.42 m for the optimal networks formed by 13 sensors, which is smaller than the averaged E_l^{10} = 19.20 m obtained with 10 sensors (Tables 2&3). The location error is observed minimum in trial 5 (E_l^{13} = 2.13 m) and maximum in trial 16 (E_l^{13} = 63.04 m) (Table 2). For this optimal network, in 80% of the trials, the source intensity is estimated within a factor of two. It was noted that the increase in the number of sensors in a network has little influence on the accuracy of the estimated intensity (Tables 2&3).

In some trials, it was also noted that the distance of an estimated source to real source can decreases with a decrease in sensors number and are also increases with the number of sensors in some other cases. It is because the information added by a new sensor was not necessarily beneficial. As it is noticeable that in a particular meteorological condition (i.e. wind direction, speed and atmospheric stability), some of the sensors in a network may have little contribution to the STE. So, increasing the number of the sensors may not always provide the best estimation because with addition of the more no. of sensors, we also add more model and measurements errors in the estimation process. These errors can affect the source estimation results in some trials. In some cases, it may also depend on sensitiveness of the added sensor's position in an extended optimal network to the source estimation. It is also noted that for a monitoring network, not only the number of sensors but also the sensors distribution form (or sensor position) affect the information captured from network.

In fact, both optimal networks for each trial show a diversity of structures independently of the number of sensors considered. For this, the *skeleton* was used to analyze the heterogeneity of the structures of different optimal networks. A skeleton with 7 sensors is considered as a strong common base for the networks. This is the case for trials 3,6,14,15&20 (Table 2). It is noted that the overall results obtained are comparable (little differences between the results obtained by the networks). For these networks, a strong common base leads to a near global optimum. If we consider networks with a weak common base, the *skeleton* was formed of up to 3 sensors, particularly in trials 1 and 11. The performances do not systematically converge independently of the size of networks. Thus, for trial 1, better results were obtained with a network formed by 13 sensors compared to that by 10 sensors. This result may reflect the fact reflects that the algorithm leading to a near global optimum is contained in with the network formed by 13 sensors, converges probably toward a near global optimum. For trial 11 also, it was noted that the performances obtained by the two networks are identical. This shows that the networks with different sensors configurations may lead to a near overall optimum. This result is in coherence with Kovalets et al. (2011) and Efthimiou et al. (2017). Considering a network of 10 sensors, they shown for the same experimental data that the best source reconstruction is possible with only 5% or 10% of the total network combinations, randomly selected.

Considering the networks of intermediate structures, with *skeletons* varying from 4 to 6 sensors, notedly for trials 2,4,5,7,8,9, 12,13,16,17,18,&19, no obvious trend is noticed. These results tend to show that for a given trial, one or more optimal networks can satisfy the conditions of a near overall optimum (to be minimized). The obtained optimal networks may have a more or less common structure (having a greater or lesser number of *skeleton*).

Moreover, uncertainties calculated for different network sizes do not show an obvious trend. Indeed, a general relationship between the number of samplers and the uncertainties is not obvious. One notice that changing size of the network (increasing or decreasing the number of sensors) can lead to the growth or diminution of the uncertainties in the source parameters estimation. As an example, for Trial 7 uncertainties grow while for Trial 17 uncertainties diminish (Table 2).

It should be noted that this study deals with the case of reducing number of sensors in order to obtain an optimal network from an existing large network. This optimization was carried out under the constraints of an existing network of the original 40 sensors in the MUST field experiment. If one compares the performances of the obtained optimal monitoring networks with the initial (original) network of 40 sensors in MUST environment, both optimal networks provide satisfactory estimations of unknown source parameters. The 40 sensors network gives an averaged location error of 14.62 m for all trials and the release rate were estimated within a factor of two in 75% trials. However, reducing the number of sensors to $1/3^{rd}$ $\sim 1/3^{rd}$ from the original 40 sensors, the 13 sensors optimal networks also give comparable source estimations performance with an averaged location error of 17.42 m. Even with the 13 sensors optimal networks, source intensities in 80% trials were accurately estimated within a factor of two. Similarly for 10 sensors optimal networks, the averaged location error (=19.20 m) is slightly larger than that obtained from 13 and 40 sensors networks. However, reducing the number of sensors to $1/4^{th}$ gives extra advantages in case of the limited available sensors for a network in emergency scenarios of an accidental or deliberated releases in complex urban environments.

Although the MUST field experiment has been widely utilized for validation of the atmospheric dispersion models and the inversion methodologies for unknown source reconstruction in an urban-like environment, its experimental domain was only approx. 200 m $\times$ 200 m (with buildings represented by a grid of containers) and can be considered small for a real urban environment. Thus, it may not quite represent a real urban region in terms of scale, meteorological variability, or non-uniform terrain or roughness/canopy structure. However, the methodology presented here is general in nature to apply to a real urban environment also. The methodology involves the utilization of the CFD model which generally can include the effects of the urban geometry, meteorological variability, or non-uniform terrain or roughness/canopy structure in a real urban environment. It is also to note that, the optimal network design would also depend on diurnal and spatial variability in meteorological conditions which may increase or decrease the optimum number of sensors and also may change the 'best positions' to be instrumented by sensors.

7 Conclusions

This study describes an approach for the optimization of a monitoring network of the sensors in a geometrically complex urban environment. It is a matter of reducing the size of networks while retaining the capabilities of detecting estimating an unknown source in an urban region. Given an urban-like environment of the MUST field experiment, the renormalization inversion method was chosen for the Source Term Estimation. It was coupled with the CFD model fluidyn-PANACHE for generation of the adjoint fields. Combinatorial optimization by the simulated annealing consisted in choosing a set of sensors which leads to an optimal monitoring network and allows an accurate unknown source estimation. This study presents the first extended an application of the renormalization data-assimilation approach theory for the definition of optimality criterion for the optimal network design to estimate an unknown continuous point release in an urban-like environment.

The numerical calculations were performed by coupling the simulated annealing stochastic algorithm to the renormalization inversion technique and the CFD modeling approach to optimize the monitoring network in urban urban-like environment of the MUST field experiment. The optimal networks enabled were constructed to reduce size of the original networks (40 sensors) to approx. one-third (13 sensors) and to one-fourth (10 sensors). The 10 and 13 sensors optimal networks have estimated the averaged location errors of 19.20 m and 17.43 m, respectively, and have comparable source estimations performance with an averaged location error of 14.62 m from the original 40 sensors network. In 80% of the trials, the emission rates with 10 and 13 sensors networks were estimated within a factor of two which are also comparable with the factor of two source intensities in 75% trials with the original network.

It was shown that in most of the MUST trials, the number of sensors in optimal networks slightly influences the location error of an estimated source and this error tends to increase as the number of sensors decreases. In 20 MUST trials, an analysis of the networks formed by 10 & 13 sensors revealed the heterogeneity of their structures in an urban domain. It was observed that for some trials, optimal networks had a strong common structure. This tends to prove that a certain number of sensors have a primordial role in determining reconstructing an unknown source. It would reflect a fact that the disjoint sets of sensors can lead to the best estimate of an unknown source in an urban region. This opens enormous prospects for assessing the relative importance of each sensor in a source reconstruction process in an urban environment. Defining a global optimal network for all meteorological conditions is a complex problem, but of greater importance that one may want to pursue. This challenge consists to define an optimal static network able to reconstruct the sources in all varied meteorological conditions. This information can be of great importance to determine an optimal monitoring network by reducing the number of sensors for characterization of the unknown emissions in the complex urban or industrial environments.

Data availability. The authors received access to the MUST field experiment dataset from Dr. Marcel Koñig of Leibniz Institute for Tropospheric Research. The MUST database was officially available from the Defense Threat Reduction Agency (DTRA) at https://must-dpg.dpg.army.mil/.

Appendix A: Weight function

Issartel et al. (2007) demonstrated that a weight function, which reduces the artifacts of the adjoint functions at the measurement points, must verify the following renormalization criterion:

$$\mathbf{a}_{\mathrm{w}}^{\mathrm{T}}(\mathbf{x})\mathbf{H}_{\mathrm{w}}^{-1}\mathbf{a}_{\mathrm{w}}(\mathbf{x}) \equiv 1 \tag{A1}$$

Following an iterative algorithm by Issartel et al. (2007), $w(\mathbf{x})$ is determined as:

$$\mathrm{w}_0(\mathbf{x}) = 1, \quad \text{and} \quad \mathrm{w}_{k+1}(\mathbf{x}) = \mathrm{w}_k(\mathbf{x})\sqrt{\mathbf{a}_{\mathrm{w}k}^{\mathrm{T}}(\mathbf{x})\mathbf{H}_{\mathrm{w}k}^{-1}\mathbf{a}_{\mathrm{w}k}(\mathbf{x})} \tag{A2}$$

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References

Abida, R.: Static and mobile networks design for atmospheric accidental releases monitoring, Theses, Ecole des Ponts ParisTech, https://pastel.archives-ouvertes.fr/pastel-00638050, 2010.

Abida, R. and Bocquet, M.: Targeting of observations for accidental atmospheric release monitoring, Atmospheric Environment, 43, 6312 – 6327, https://doi.org/http://dx.doi.org/10.1016/j.atmosenv.2009.09.029, http://www.sciencedirect.com/science/article/pii/S1352231009008048, 2009.

Abida, R., Bocquet, M., Vercauteren, N., and Isnard, O.: Design of a monitoring network over France in case of a radiological accidental release, Atmospheric Environment, 42, 5205 – 5219, https://doi.org/http://dx.doi.org/10.1016/j.atmosenv.2008.02.065, http://www.sciencedirect.com/science/article/pii/S1352231008002409, 2008.

Beljaars, A. and Holtslag, A.: Flux parameterization over land surfaces for atmospheric models, Journal of Applied Meteorology, 30, 327–341, https://doi.org/10.1175/1520-0450(1991)030<0327:FPOLSF>2.0.CO;2, http://dx.doi.org/10.1175/1520-0450(1991)030<0327:FPOLSF>2.0.CO;2, 1991.

Biltoft, C. A.: Customer Report for Mock Urban Setting Test, Tech. rep., West Desert Test Center, U.S. Army Dugway Proving Ground, Dugway, Utah, 2001.

Bocquet, M.: Reconstruction of an atmospheric tracer source using the principle of maximum entropy. I: Theory, Quarterly Journal of the Royal Meteorological Society, 131, 2191–2208, https://doi.org/10.1256/qj.04.67, http://dx.doi.org/10.1256/qj.04.67, 2005.

Cohn, H. and Fielding, M.: Simulated Annealing: Searching for an Optimal Temperature Schedule, SIAM Journal on Optimization, 9, 779–802, https://doi.org/10.1137/S1052623497329683, https://doi.org/10.1137/S1052623497329683, 1999.

Efthimiou, G. C., Kovalets, I. V., Venetsanos, A., Andronopoulos, S., Argyropoulos, C. D., and Kakosimos, K.: An optimized inverse modelling method for determining the location and strength of a point source releasing airborne material in urban environment, Atmospheric Environment, 170, 118 – 129, https://doi.org/https://doi.org/10.1016/j.atmosenv.2017.09.034, http://www.sciencedirect.com/science/article/pii/S1352231017306337, 2017.

Gamerman, D. and Lopes, H. F.: Markov chain Monte Carlo: stochastic simulation for Bayesian inference, CRC Press, 2006.

Gryning, S.-E., Batchvarova, E., Brummer, B., Jorgensen, H., and Larsen, S.: On the extension of the wind profile over homogeneous terrain beyond the surface boundary layer, Boundary-Layer Meteorology, 124, 251–268, https://doi.org/10.1007/s10546-007-9166-9, http://dx.doi.org/10.1007/s10546-007-9166-9, 2007.

Haupt, S. E., Young, G. S., and Allen, C. T.: Validation of a receptor-dispersion model coupled with a genetic algorithm using synthetic data, Journal of applied meteorology and climatology, 45, 476–490, https://doi.org/10.1175/JAM2359.1, http://dx.doi.org/10.1175/JAM2359.1, 2006.

Hourdin, F. and Talagrand, O.: Eulerian backtracking of atmospheric tracers. I: Adjoint derivation and parametrization of subgrid-scale transport, Quarterly Journal of the Royal Meteorological Society, 132, 567–583, https://doi.org/10.1256/qj.03.198.A, http://dx.doi.org/10.1256/qj.03.198.A, 2006.

Hutchinson, M., Oh, H., and Chen, W.-H.: A review of source term estimation methods for atmospheric dispersion events using static or mobile sensors, Information Fusion, 36, 130 – 148, https://doi.org/https://doi.org/10.1016/j.inffus.2016.11.010, http://www.sciencedirect.com/science/article/pii/S156625351630152X, 2017.

Issartel, J.-P.: Emergence of a tracer source from air concentration measurements, a new strategy for linear assimilation, Atmospheric Chemistry and Physics, 5, 249–273, https://doi.org/10.5194/acp-5-249-2005, http://www.atmos-chem-phys.net/5/249/2005/, 2005.

Issartel, J.-P., Sharan, M., and Modani, M.: An inversion technique to retrieve the source of a tracer with an application to synthetic satellite measurements, Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, 463, 2863–2886, https://doi.org/10.1098/rspa.2007.1877, http://rspa.royalsocietypublishing.org/content/463/2087/2863.abstract, 2007.

Issartel, J.-P., Sharan, M., and Singh, S. K.: Identification of a Point of Release by Use of Optimally Weighted Least Squares, Pure and Applied Geophysics, 169, 467–482, https://doi.org/10.1007/s00024-011-0381-4, https://doi.org/10.1007/s00024-011-0381-4, 2012.

Jiang, Z., de Bruin, S., Heuvelink, G., and Twenhöfel, C.: Optimization of mobile radioactivity monitoring networks, http://edepot.wur.nl/24174, 2007.

Keats, W. A.: Bayesian inference for source determination in the atmospheric environment, Ph.D. thesis, http://hdl.handle.net/10012/4317, 2009.

Kirkpatrick, S., Gelatt, C. D., and Vecchi, M. P.: Optimization by Simulated Annealing, Science, 220, 671–680, https://doi.org/10.1126/science.220.4598.671, http://science.sciencemag.org/content/220/4598/671, 1983.

Ko, C.-W., Lee, J., and Queyranne, M.: An Exact Algorithm for Maximum Entropy Sampling, Operations Research, 43, 684–691, https://doi.org/10.1287/opre.43.4.684, https://doi.org/10.1287/opre.43.4.684, 1995.

Kouichi, H.: Sensors networks optimization for the characterization of atmospheric releases source, Theses, Université Paris Saclay, France, https://hal.archives-ouvertes.fr/tel-01593834, 2017.

Kouichi, H., Turbelin, G., Ngae, P., Feiz, A., Barbosa, E., and Chpoun, A.: Optimization of sensor networks for the estimation of atmospheric pollutants sources, WIT Transactions on Ecology and the Environment, 207, 11–21, 2016.

Kovalets, I. V., Andronopoulos, S., Venetsanos, A. G., and Bartzis, J. G.: Identification of strength and location of stationary point source of atmospheric pollutant in urban conditions using computational fluid dynamics model, Mathematics and Computers in Simulation, 82, 244 – 257, https://doi.org/http://dx.doi.org/10.1016/j.matcom.2011.07.002, http://www.sciencedirect.com/science/article/pii/S0378475411001686, 2011.

Kumar, P., Feiz, A.-A., Ngae, P., Singh, S. K., and Issartel, J.-P.: CFD simulation of short-range plume dispersion from a point release in an urban like environment, Atmospheric Environment, 122, 645 – 656, https://doi.org/http://dx.doi.org/10.1016/j.atmosenv.2015.10.027, http://www.sciencedirect.com/science/article/pii/S1352231015304465, 2015a.

Kumar, P., Feiz, A.-A., Singh, S. K., Ngae, P., and Turbelin, G.: Reconstruction of an atmospheric tracer source in an urban-like environment, Journal of Geophysical Research: Atmospheres, 120, 12 589–12 604, https://doi.org/10.1002/2015JD024110, http://dx.doi.org/10.1002/2015JD024110, 2015b.

Kumar, P., Singh, S. K., Feiz, A.-A., and Ngae, P.: An urban scale inverse modelling for retrieving unknown elevated emissions with building-resolving simulations, Atmospheric Environment, 140, 135 – 146, https://doi.org/http://dx.doi.org/10.1016/j.atmosenv.2016.05.050, http://www.sciencedirect.com/science/article/pii/S1352231016303983, 2016.

Ma, D., Deng, J., and Zhang, Z.: Comparison and improvements of optimization methods for gas emission source identification, Atmospheric Environment, 81, 188 – 198, https://doi.org/https://doi.org/10.1016/j.atmosenv.2013.09.012, http://www.sciencedirect.com/science/article/pii/S1352231013007000, 2013.

Ma, D., Tan, W., Zhang, Z., and Hu, J.: Parameter identification for continuous point emission source based on Tikhonov regularization method coupled with particle swarm optimization algorithm, Journal of Hazardous Materials, 325, 239 – 250, https://doi.org/https://doi.org/10.1016/j.jhazmat.2016.11.071, http://www.sciencedirect.com/science/article/pii/S0304389416311141, 2017.

Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H., and Teller, E.: Equation of State Calculations by Fast Computing Machines, The Journal of Chemical Physics, 21, 1087–1092, https://doi.org/10.1063/1.1699114, https://doi.org/10.1063/1.1699114, 1953.

Monache, L. D., Lundquist, J. K., Kosović, B., Johannesson, G., Dyer, K. M., Aines, R. D., Chow, F. K., Belles, R. D., Hanley, W. G., Larsen, S. C., Loosmore, G. A., Nitao, J. J., Sugiyama, G. A., and Vogt, P. J.: Bayesian Inference and Markov Chain Monte Carlo Sampling to Reconstruct a Contaminant Source on a Continental Scale, Journal of Applied Meteorology and Climatology, 47, 2600–2613, https://doi.org/10.1175/2008JAMC1766.1, https://doi.org/10.1175/2008JAMC1766.1, 2008.

Nourani, Y. and Andresen, B.: A comparison of simulated annealing cooling strategies, Journal of Physics A: Mathematical and General, 31, 8373, http://stacks.iop.org/0305-4470/31/i=41/a=011, 1998.

Penenko, V., Baklanov, A., and Tsvetova, E.: Methods of sensitivity theory and inverse modeling for estimation of source parameters, Future Generation Computer Systems, 18, 661 – 671, https://doi.org/http://dx.doi.org/10.1016/S0167-739X(02)00031-6, http://www.sciencedirect.com/science/article/pii/S0167739X02000316, {ICCS2001}, 2002.

Pudykiewicz, J. A.: Application of adjoint tracer transport equations for evaluating source parameters, Atmospheric Environment, 32, 3039–3050, https://doi.org/http://dx.doi.org/10.1016/S1352-2310(97)00480-9, http://www.sciencedirect.com/science/article/pii/S1352231097004809, 1998.

Qu, Y., Milliez, M., Musson-Genon, L., and Carissimo, B.: Micrometeorological Modeling of Radiative and Convective Effects with a Building-Resolving Code, Journal of Applied Meteorology and Climatology, 50, 1713–1724, https://doi.org/10.1175/2011JAMC2620.1, https://doi.org/10.1175/2011JAMC2620.1, 2011.

Rao, K. S.: Source estimation methods for atmospheric dispersion, Atmospheric Environment, 41, 6964 – 6973, https://doi.org/https://doi.org/10.1016/j.atmosenv.2007.04.064, http://www.sciencedirect.com/science/article/pii/S1352231007004086, 2007.

Saunier, O., Bocquet, M., Mathieu, A., and Isnard, O.: Model reduction via principal component truncation for the optimal design of atmospheric monitoring networks, Atmospheric Environment, 43, 4940 – 4950, https://doi.org/http://dx.doi.org/10.1016/j.atmosenv.2009.07.011, http://www.sciencedirect.com/science/article/pii/S1352231009005913, 2009.

Seibert, P.: Inverse Modelling with a Lagrangian Particle Disperion Model: Application to Point Releases Over Limited Time Intervals, pp. 381–389, Springer US, Boston, MA, https://doi.org/10.1007/0-306-47460-3_38, https://doi.org/10.1007/0-306-47460-3_38, 2001.

Seibert, P. and Frank, A.: Source-receptor matrix calculation with a Lagrangian particle dispersion model in backward mode, Atmospheric Chemistry and Physics, 4, 51–63, 2004.

Sharan, M., Issartel, J.-P., Singh, S. K., and Kumar, P.: An inversion technique for the retrieval of single-point emissions from atmospheric concentration measurements, Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, 465, 2069–2088, https://doi.org/10.1098/rspa.2008.0402, http://rspa.royalsocietypublishing.org/content/early/2009/04/09/rspa.2008.0402.abstract, 2009.

Sharan, M., Singh, S. K., and Issartel, J.-P.: Least Square Data Assimilation for Identification of the Point Source Emissions, Pure and Applied Geophysics, 169, 483–497, https://doi.org/10.1007/s00024-011-0382-3, http://dx.doi.org/10.1007/s00024-011-0382-3, 2012.

Siarry, P.: Métaheuristiques: Recuits simulé, recherche avec tabous, recherche à voisinages variables, méthodes GRASP, algorithmes évolutionnaires, fourmis artificielles, essaims particulaires et autres méthodes d'optimisation, Editions Eyrolles, 2014.

Siarry, P.: Simulated Annealing, pp. 19–50, Springer International Publishing, Cham, https://doi.org/10.1007/978-3-319-45403-0_2, http://dx.doi.org/10.1007/978-3-319-45403-0_2, 2016.

Wang, B., Chen, B., and Zhao, J.: The real-time estimation of hazardous gas dispersion by the integration of gas detectors, neural network and gas dispersion models, Journal of Hazardous Materials, 300, 433 – 442, https://doi.org/http://dx.doi.org/10.1016/j.jhazmat.2015.07.028, http://www.sciencedirect.com/science/article/pii/S0304389415005658, 2015.

Yang, Y., Gu, M., Chen, S., and Jin, X.: New inflow boundary conditions for modelling the neutral equilibrium atmospheric boundary layer in computational wind engineering, Journal of Wind Engineering and Industrial Aerodynamics, 97, 88–95, https://doi.org/http://dx.doi.org/10.1016/j.jweia.2008.12.001, http://www.sciencedirect.com/science/article/pii/S0167610508001815, 2009.

Yee, E. and Biltoft, C.: Concentration Fluctuation Measurements in a Plume Dispersing Through a Regular Array of Obstacles, Boundary-Layer Meteorology, 111, 363–415, https://doi.org/10.1023/B:BOUN.0000016496.83909.ee, http://dx.doi.org/10.1023/B%3ABOUN.0000016496.83909.ee, 2004.

Yee, E., Hoffman, I., and Ungar, K.: Bayesian Inference for Source Reconstruction: A Real-World Application, International Scholarly Research Notices, 2014, 1–12, https://doi.org/10.1155/2014/507634, http://dx.doi.org/10.1155/2014/507634, 2014.

Zhang, X., Raskob, W., Landman, C., Trybushnyi, D., and Li, Y.: Sequential multi-nuclide emission rate estimation method based on gamma dose rate measurement for nuclear emergency management, Journal of Hazardous Materials, 325, 288 – 300, https://doi.org/https://doi.org/10.1016/j.jhazmat.2016.10.072, http://www.sciencedirect.com/science/article/pii/S0304389416310032, 2017.

Zhang, X. L., Su, G. F., Yuan, H. Y., Chen, J. G., and Huang, Q. Y.: Modified ensemble Kalman filter for nuclear accident atmospheric dispersion: Prediction improved and source estimated, Journal of Hazardous Materials, 280, 143 – 155, https://doi.org/https://doi.org/10.1016/j.jhazmat.2014.07.064, http://www.sciencedirect.com/science/article/pii/S0304389414006396, 2014.

Zhang, X. L., Su, G. F., Chen, J. G., Raskob, W., Yuan, H. Y., and Huang, Q. Y.: Iterative ensemble Kalman filter for atmospheric dispersion in nuclear accidents: An application to Kincaid tracer experiment, Journal of Hazardous Materials, 297, 329 – 339, https://doi.org/https://doi.org/10.1016/j.jhazmat.2015.05.035, http://www.sciencedirect.com/science/article/pii/S0304389415004318, 2015.

Table 1. The values of the meteorological (wind speed (S_{04}), wind direction (α_{04}) at 4 m level of mast S), turbulence (the Obukhov length (L), friction velocity (u_*), turbulent kinetic energy (k) at 4 m level of tower T), and source parameters (source height (z_s), release duration (t_s), release rate (q_s)) in 20 selected trials of the MUST field experiment (Biltoft, 2001; Yee and Biltoft, 2004). Here, Trial Nos. 1-20 are assigned for just continuation and simplicity and these are not correspond to the same assigned trial no. for a given Trial name in the MUST experiment.

Trial No.	Trial Name (JJJhhmm)	q_s (l/min)	t_s (min)	z_s (m)	S_{04} (m/s)	α_{04} (deg)	u_* (m/s)	L (m)	k (m^2s^{-2})
1	2640138	175	21	0.15	2.35	17	0.26	91	0.359
2	2640246	200	15	0.15	2.01	30	0.25	62	0.306
3	2671852	200	22	0.15	3.06	-49	0.32	330	0.436
4	2671934	200	15	1.8	1.63	-48	0.08	5.8	0.148
5	2672033	200	15	1.8	2.69	-26	0.17	4.8	0.251
6	2672101	200	14	0.15	1.89	-10	0.16	7.7	0.218
7	2672150	200	16	0.15	2.30	36	0.35	150	0.409
8	2672213	200	15	1.8	2.68	30	0.35	150	0.428
9	2672235	200	15	2.6	2.32	36	0.26	48	0.387
10	2672303	200	19	1.8	2.56	17	0.25	74	0.367
11	2681829	225	15	1.8	7.93	-41	1.10	28000	1.46
12	2681849	225	16	0.15	7.26	-50	0.76	2500	0.877
13	2682256	225	15	0.15	5.02	-42	0.66	240	0.877
14	2682320	225	15	2.6	4.55	-39	0.50	170	0.718
15	2682353	225	15	5.2	4.49	-47	0.44	120	0.727
16	2692054	225	22	1.3	3.34	39	0.36	170	0.362
17	2692131	225	17	1.3	4.00	39	0.42	220	0.582
18	2692157	225	15	2.6	2.98	43	0.39	130	0.505
19	2692223	225	15	1.3	2.63	26	0.35	120	0.484
20	2692250	225	17	1.3	3.38	36	0.37	130	0.537

Table 2. Source estimation results from the different monitoring networks for each selected trial of the MUST field experiment. E_l^p and E_q^p respectively denote the location error (m) and ratio of the estimated to true source intensity with the corresponding monitoring network. Here, the superscript p on E_l^p & E_q^p represents the no. of sensors in an optimal network. *Skeleton* refers to the number of sensors common to the optimal networks of 10 and 13 sensors for a given MUST trial.

Run No.	E_l^{40} (m)	E_l^{13} (m)	E_l^{10} (m)	E_q^{40}	E_q^{13}	E_q^{10}	*Skeleton* sensors
1	3.3±1.3	19.6 19.60±12.13	33.76±5.30	0.92±0.08	1.04±0.23	1.24±0.22	3
2	42.9±23.8	31.91±8.80	56.88±9.51	4.01±1.57	3.21±0.41	5.12±3.63	4
3	10.8±1.6	9.01±2.47	9.01±3.02	1.17±0.27	0.71±0.16	0.71±0.16	7
4	22.8±7.7	18.07±1.84	18.07±2.61	0.27±0.35	0.83±0.21	0.83±0.26	6
5	21.9±2.1	2.13±2.54	11.56±4.21	0.57±0.07	0.95±0.05	0.67±0.05	6
6	5.0±1.6	6.96±0.19	6.96±0.00	2.14±0.60	1.04±0.06	1.04±0.04	7
7	12.4±9.1	18.85±9.08	12.99±1.67	0.41±0.49	3.11±0.51	1.06±0.07	4
8	15.8±12.1	12.86±1.28	15.79±1.05	2.22±0.90	1.32±0.34	1.76±0.11	6
9	7.7±1.2	8.20±0.35	8.08±0.00	1.37±0.07	3.06±0.17	7.55±0.39	5
10	8.8±3.0	8.00±4.57	8.00±5.68	1.08±0.19	1.08±0.77	1.08±1.07	8
11	19.8±5.0	17.19±12.00	17.19±7.06	1.67±0.12	1.62±0.40	1.62±0.26	3
12	7.4±6.6	5.43±11.69	10.22±9.10	0.95±0.06	0.85±0.28	0.2 0.20±0.04	4
13	7.7±0.6	8.63±4.36	8.63±3.86	0.97±0.07	0.78±0.18	0.78±2.05	4
14	2.2±1.9	5.50±2.98	5.50±3.88	1.42±0.17	0.88±0.24	0.88±0.40	7
15	1.1±1.0	30.23±2.14	37.98±0.72	1.88±0.09	0.57±0.07	0.17±0.01	7
16	26.7±4.9	63.04±6.84	29.80±9.86	1.70±0.06	0.29±0.06	0.67±0.23	5
17	7.0±1.9	14.07±2.78	23.05±10.44	0.90±0.05	1.10±0.04	1.52±0.16	6
18	14.3±11.0	12.83±4.18	12.83±4.61	1.15±0.46	1.15±0.16	1.15±0.21	6
19	22.3±6.4	10.77±4.25	13.46±4.8	1.76±0.16	0.99±0.20	0.83±0.25	6
20	32.5±1.8	45.23±1.78	44.29±0.31	0.83±0.04	1.68±0.06	1.56±0.06	7

Table 3. Statistics for the source reconstruction results from each monitoring network. Here, E_l^p is the averaged location error for all 20 trials corresponding to each network. FAg represents the percentage number of trials in which the source intensity is estimated within a factor of g.

Sensors (p)	E_l^p **(m)**	**FA4**	**FA3**	**FA2**
40	14.62	95	90	75
13	17.42	100	80	80
10	19.20	80	80	80

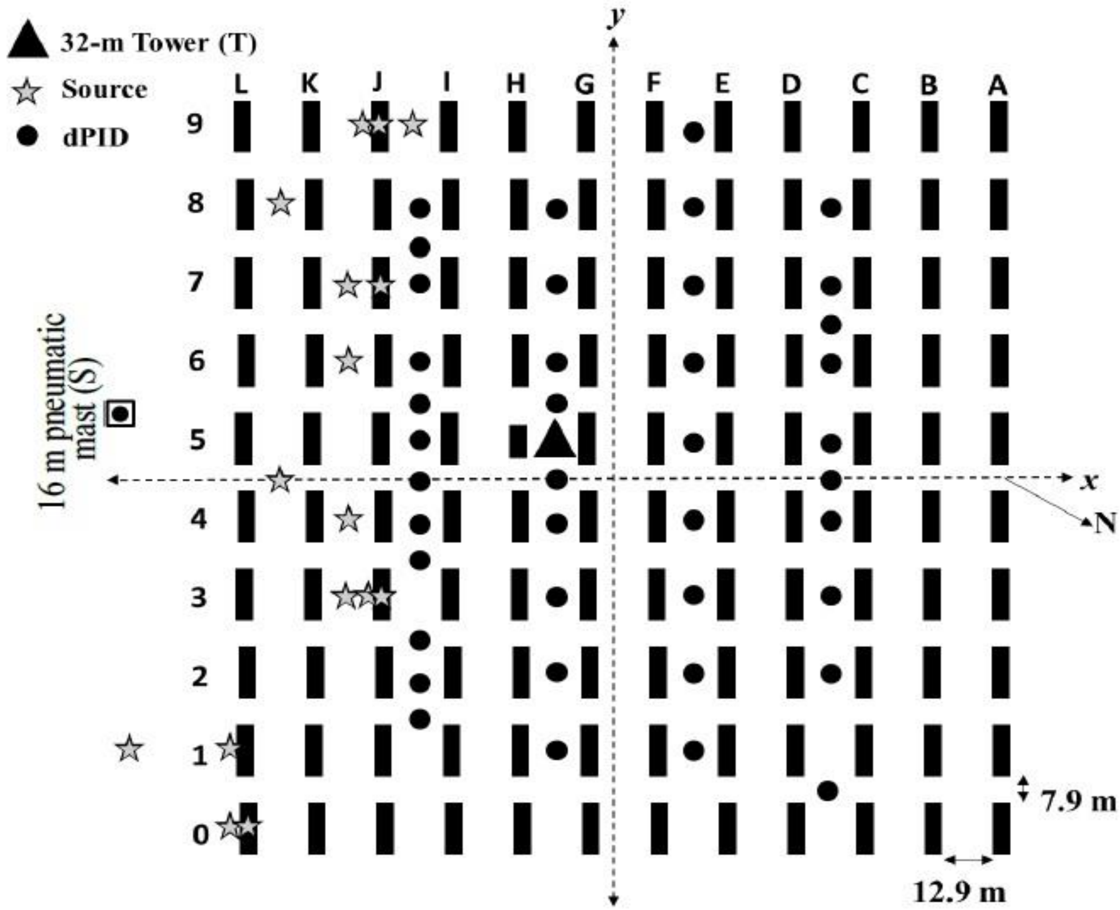

Figure 1. A schematic diagram of the MUST geometry showing 120 containers and source (stars) and receptors (black filled circles) locations. In a given trial - only one source was operational.

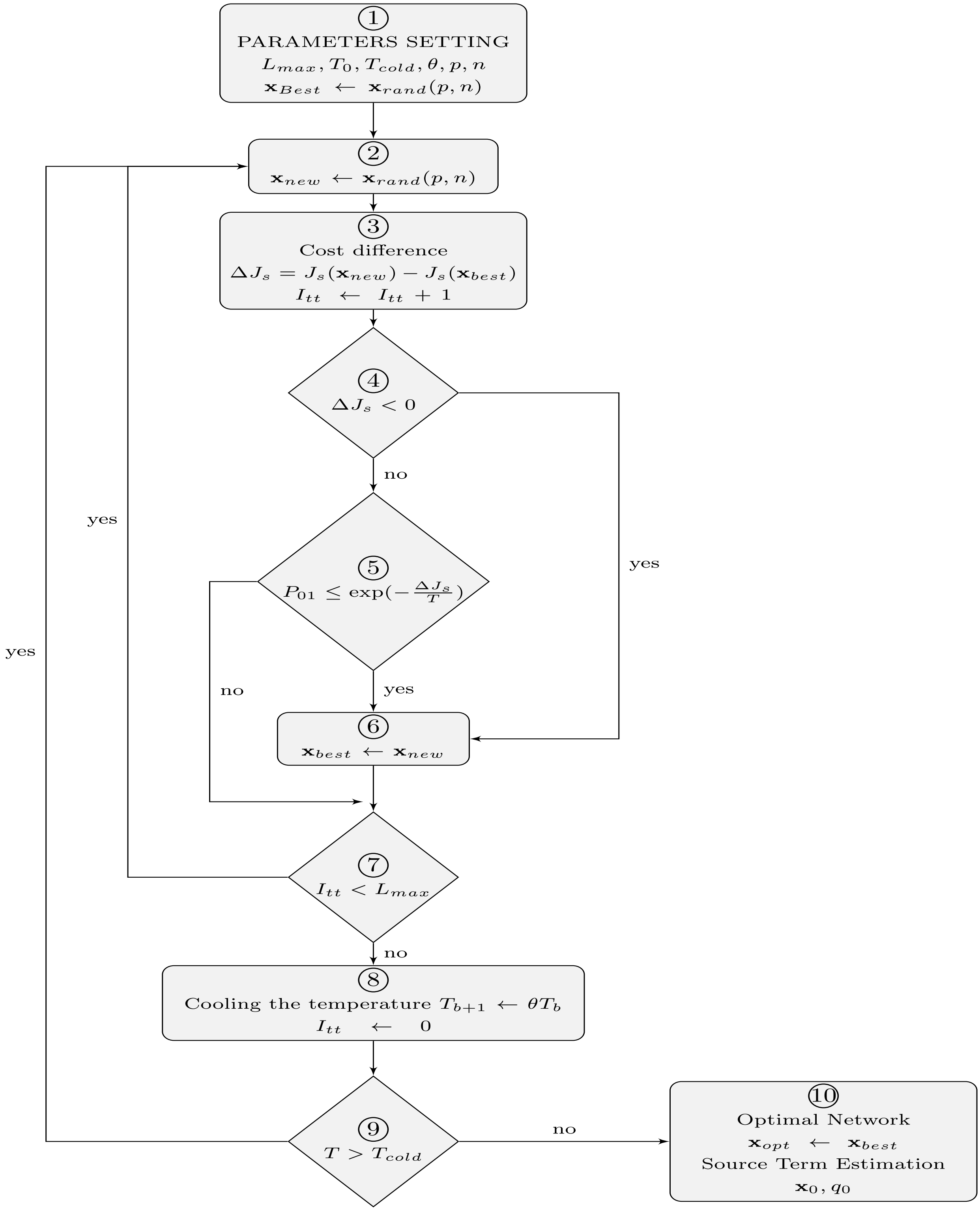

Figure 2. Flow diagram of the Simulated Annealing procedures to determine an optimized monitoring network.

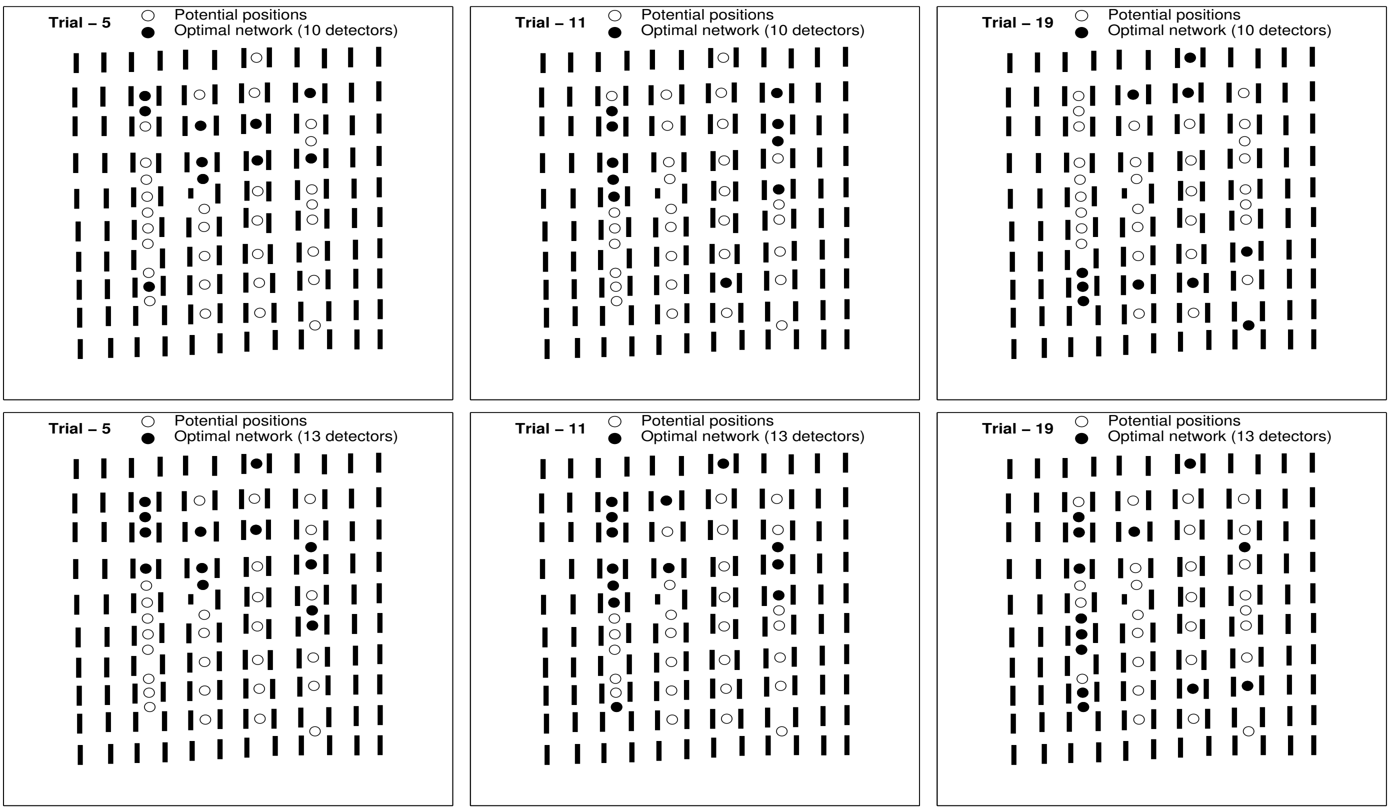

Figure 3. The optimal networks of 10 (first row) and 13 sensors (second row) respectively for trials 5 (very stable), 11 (neutral), and 19 (stable). Blank and filled black circles respectively represent the all (40) potential positions and the optimal positions of sensors.

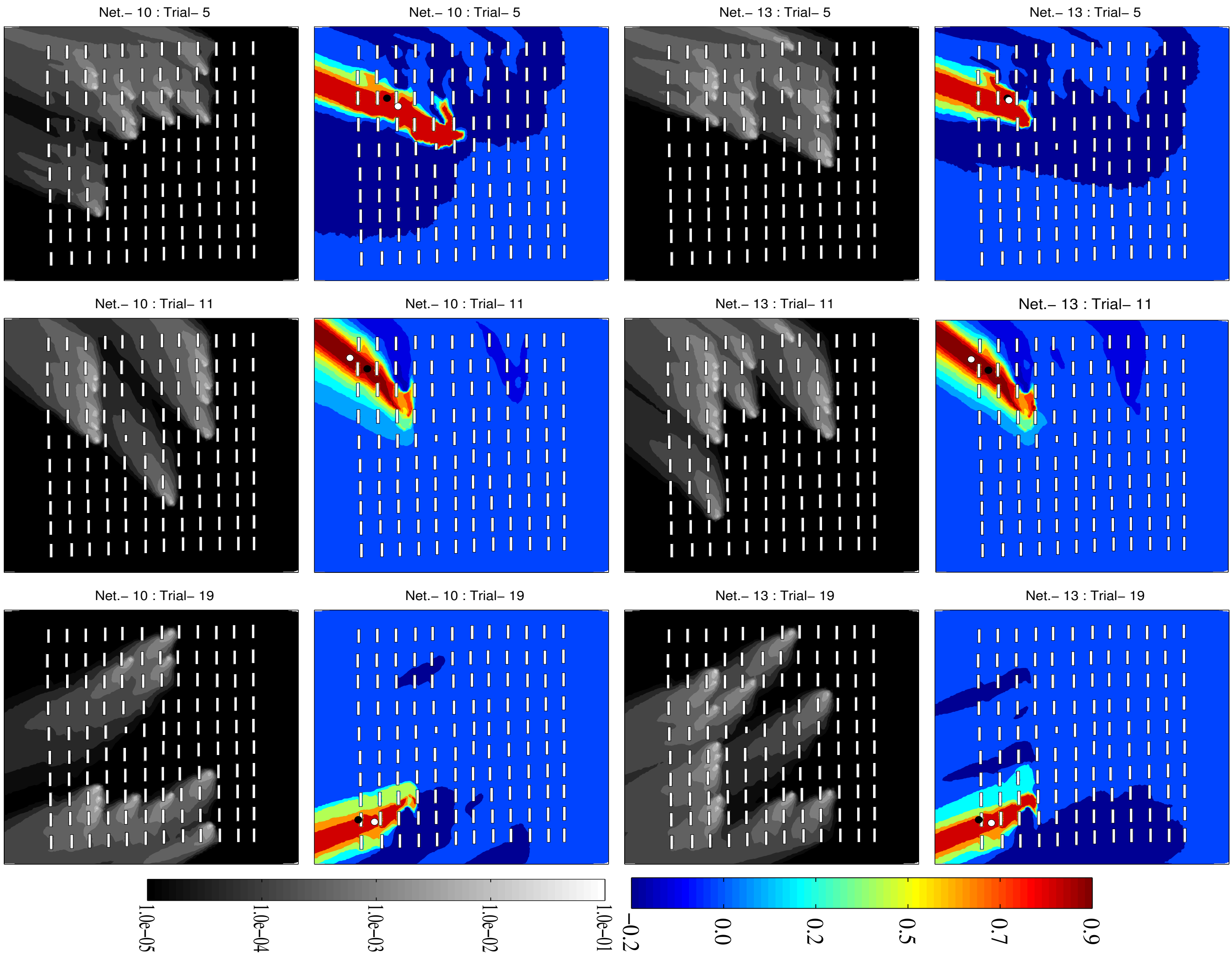

Figure 4. Isopleths of the renormalized weight function $(w(\mathbf{x}))$ (gray colored in first and third columns) and the normalized source estimate function $(\mathbf{s}_w^n(\mathbf{x}) = \mathbf{s}_w(\mathbf{x})/\max(\mathbf{s}_w(\mathbf{x})))$ (colored in second and fourth columns) for both optimal networks of 10 and 13 sensors respectively for trials 5 (very stable), 11 (neutral), and 19 (stable). The black and white filled circles respectively represent the true and estimated source locations.