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 suggestions, the manuscript is revised. Reviewer's questions and remarks are repeated below (in red color) and our responses follow each question (in italic).

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 atmospheric stratification through surface coolingor 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 specification of the stability dependent inflow boundary conditions only, the predicting concentrations from the CFD model are in goodagreement with the measured concentrationsin the MUST experimentfor 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 enoughfor the requirement to resolve theatmospheric stratification through surface coolingor 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. Andthe stability effects through the specification of inflow boundary conditionsonly may not be appropriate for those environments. In these scenarios, the CFD model should be capable of incorporating the atmospheric stratification through surface coolingor 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 urbanenvironments. 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 remarksthat 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 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 for 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 arbitrary. 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 be 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.*

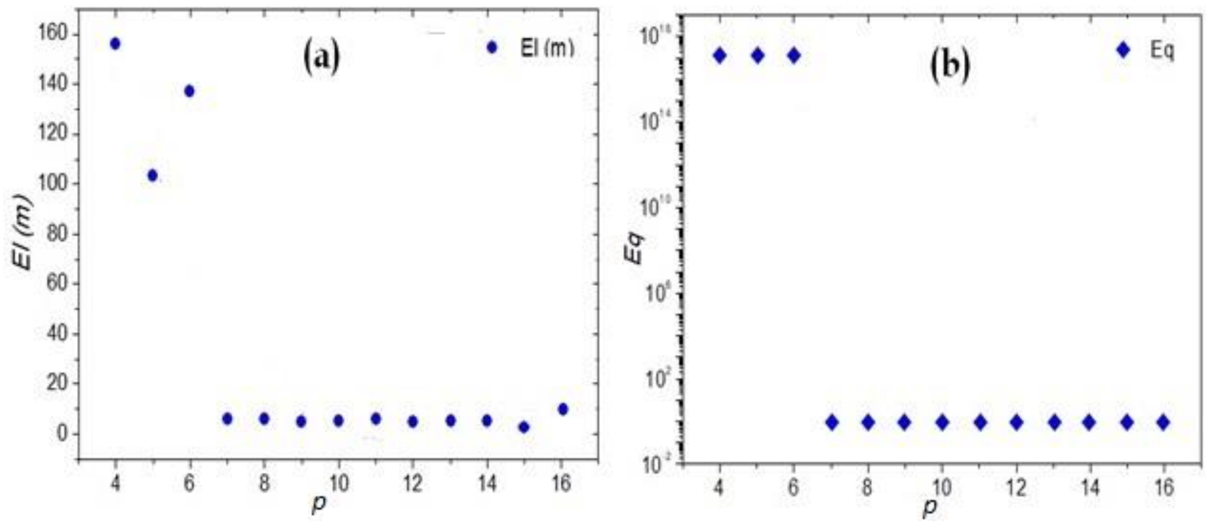

Figure 1: Errors in the estimation of the source (a) position and (b) intensity in Trial 14. Here p is the number of sensors

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 a 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 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 measurements. 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 result are present in the 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 the size of network (increasing or decreasing the number of sensors) can lead to the growth or diminution of the uncertainties in the source parameters estimation. As 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 artefacts 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 an operational 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 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 assumptions with respectto the vertical structure of the problem is useful to estimate the ground level sources or the emission sourcesalong a horizontal cross-section area passing through a fixed vertical level. However, in this study, the problem of vertical structure (i.e. 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 revised 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.*

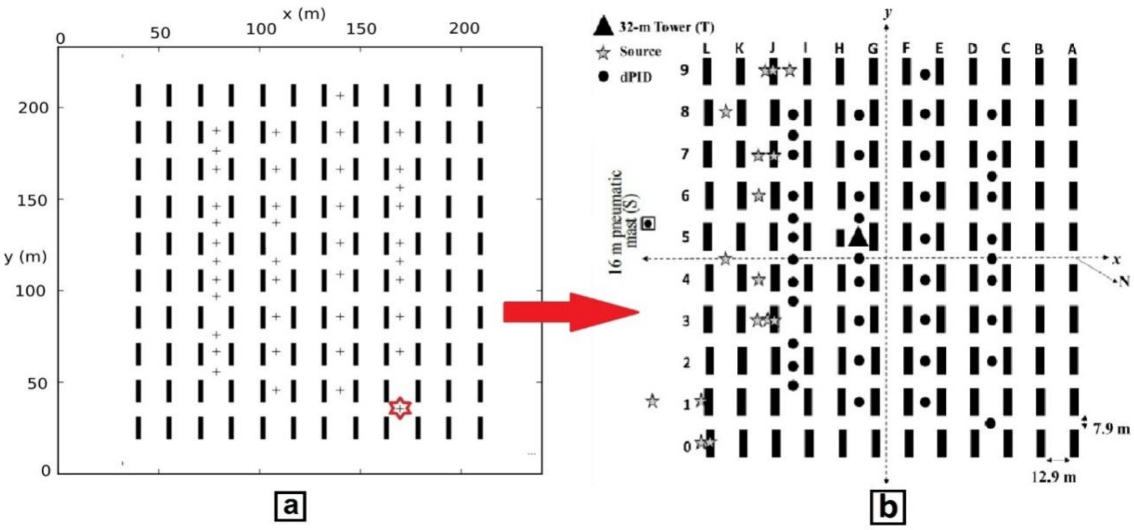

Figure 2: Schematization of the MUST experiment: (a) correct version (b) adjusted version

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

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

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