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.*

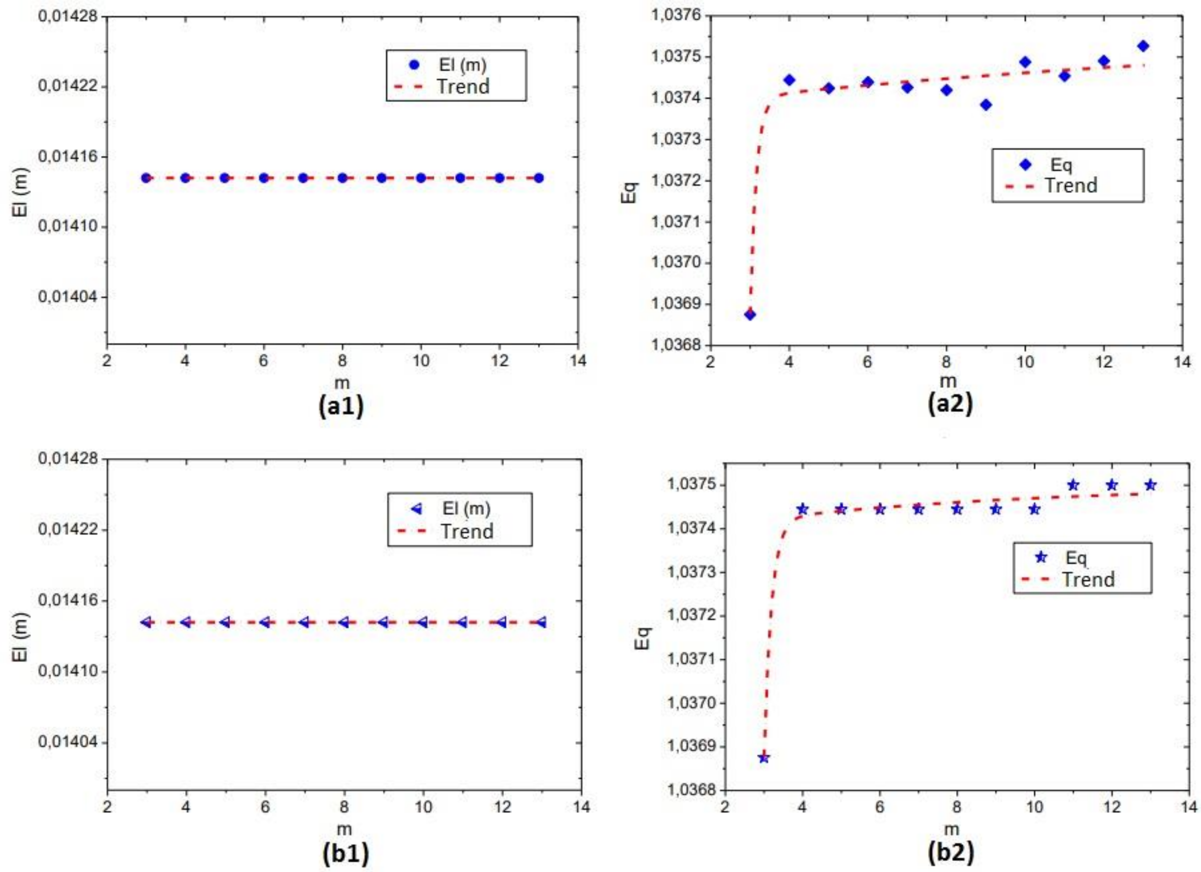

Figure 1: Error of source parameters estimation for (a) SA (b) GA in the DYCE wind tunnel experiment. Here m is the number of sensors, E_l and E_q respectively denote the location error (m) and the ratio of the estimated to true source intensity

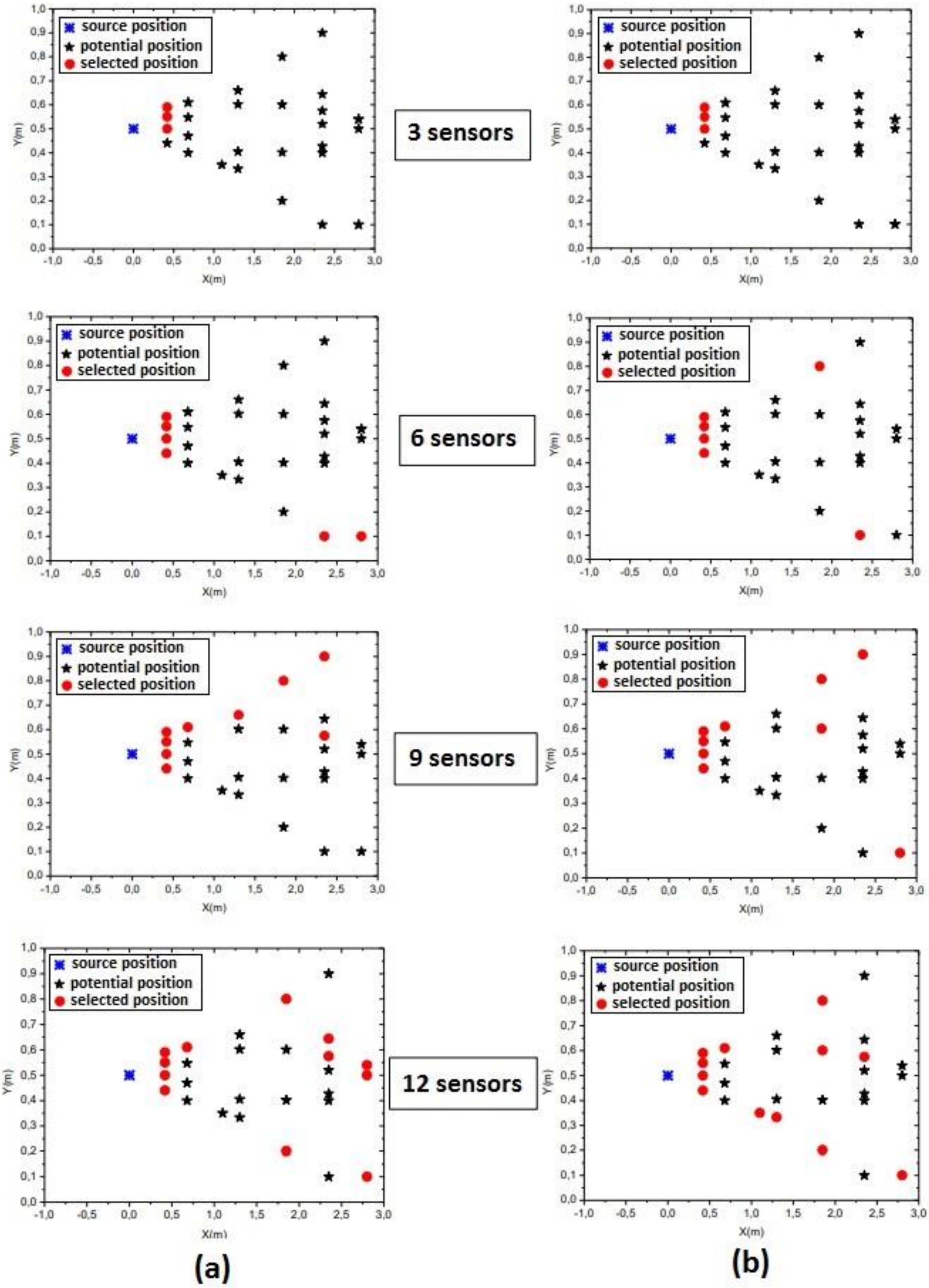

Figure 2: Optimal networks (m = 3, 6, 9 and 12) obtained by (a) Simulated Annealing SA and (b) Genetic Algorithm GA

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.*

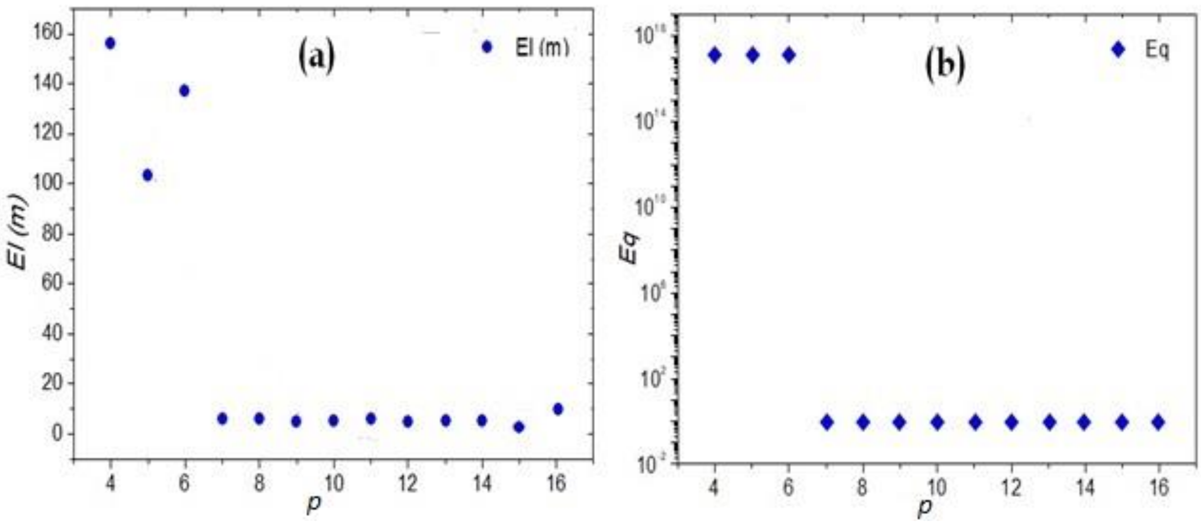

Figure 3: Errors in the estimation of the source (a) position and (b) intensity in Trial 14. Here p is the number of sensors

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.

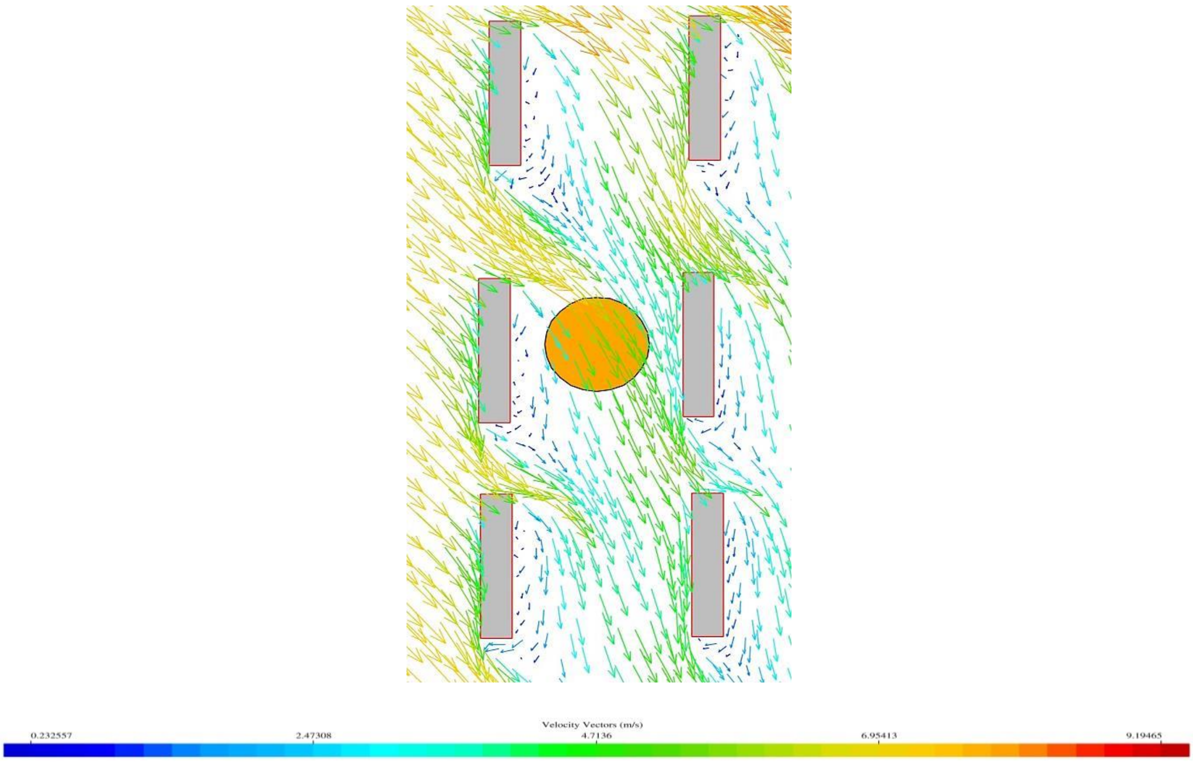

Figure 4: Wind velocity vectors for the trial 11

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