INVERSE IDENTIFICATION OF UNKNOWN STATIONARY AIR POLLUTANT RELEASE FROM A POINT SOURCE IN URBAN ENVIRONMENT

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ABSTRACT
An improved inverse modelling method to estimate the location and the emission rate of an unknown point stationary source of passive atmospheric pollutant in a complex urban geometry was incorporated in the Computational Fluid Dynamics code ADREA-HF in Efthimiou et al., (2017). The key improvement lies in a two-step segregated approach. At first only the source coordinates are analysed using a correlation function of measured and calculated concentrations. In the second step the source rate is identified by minimizing a quadratic cost function. The validation of the algorithm was performed by simulating three wind tunnel experiments: the MUST, Michelstadt and Complex Urban Terrain Experiment (CUTE). The method appears to be robust and to predict with encouraging accuracy the source location and emission rate for all wind tunnel experiments. A discussion is given in the paper about the possible practicability of the method for emergency response.

Keywords: Inverse modelling; Source term estimation; CFD; ADREA-HF; Urban environment; Source inversion; Emergency response.

1. INTRODUCTION

In the event of a dangerous substance being released into the atmosphere, whether intentionally or by accident, the transport of the material as a wind-blown plume can distribute it over a large area and may pose threats to the populations in the course of the plume.

The Chernobyl (Anspaugh et al., 1988), and relatively recent Fukushima (Ohtsuru et al., 2015) nuclear disasters are significant events which caused severe environmental and human health and life consequences.

During an event of the type described above and if the source location, the release rate and type of pollutants are known, dispersion models can be used to forecast the plume trajectory of the air pollutants, their dispersion and eventual deposition as well as the level of human exposure to the pollutant(s). The necessary meteorological information may originate from local weather stations or may be forecast data provided by Numerical Weather Prediction models. If the source characteristics, such as location, release rate and pollutant type (collectively mentioned as “source term”) are unknown and the only available information is readings at different locations and time intervals, the reconstruction of the source term of the airborne pollutant can usually be obtained by using forward or backward (inverse) modelling approaches, in combination with the existing measurements.

Important research has been performed in developing methods for the identification of the unknown source of an airborne material. Various researchers have tried to combine inverse modelling techniques with the Computational Fluid Dynamics (CFD) (either Reynolds-Averaged Navier-Stokes (RANS), Efthimiou et al., 2017; Efthimiou et al., 2018 or Large Eddy Simulation (LES), Mons et al., 2017).

Recently, Efthimiou et al. (2017) exhibited an optimized inverse modelling method for the reconstruction of pollutant stationary source characteristics in urban environment. The method eliminates the 'overfitting' effect by determining the source location and rate separately, through a two-step segregated approach that combines a correlation coefficient and a cost function. The method was recently extended by Kovalets et al., (2018) for the case of transient dispersion problem.

This paper presents some of the results of Efthimiou et al. (2017) and Efthimiou et al. (2018) as well as presents the new efforts of authors to extend the applicability of the method for emergency response situations. Section 2 presents the inverse methodology and Section 3 the examined experiments that were used to validate the model. Then Section 4 presents the results. Finally, Section 5 provides a discussion about the possible usage of the methodology for emergency response and in Section 6 some major conclusions are given. A description of the numerical simulations can be found in Efthimiou et al. (2017) and Efthimiou et al. (2018).

2. METHODOLOGY – SOURCE TERM ESTIMATION ALGORITHM

The first version of the inverse source term estimation algorithm was described by Kovalets et al., (2011) and the optimised version that is used in this paper has been described by Efthimiou et al., (2017). The outline and the basic relationships of the algorithm will be given here.

The basic assumptions of the problem are that there is a constant-in-time air flow field established over an urban area, into which a pollutant is emitted at a constant rate from a point source. The steady-state flow field is calculated by a CFD model. Besides the steady-state flow field, the only available information is concentration measurements at several sensors' locations inside the urban area under consideration. The source can be located anywhere in the computational domain. The location of the source is estimated by calculating and finding the minimum of the following cost function:

$$J = -\frac{\left\langle \left(c^c - \left\langle c^c \right\rangle\right)\left(c^o - \left\langle c^o \right\rangle\right)\right\rangle}{\sqrt{\left\langle \left(c^c - \left\langle c^c \right\rangle\right)^2 \right\rangle}\sqrt{\left\langle \left(c^o - \left\langle c^o \right\rangle\right)^2 \right\rangle}} \tag{1}$$

where c^c indicates calculated and c^o indicates observed concentration respectively, both at the sensor's locations and $\langle \ \rangle$ denotes arithmetic averaging over all sensors positions. The function J is minimized with respect to the source location, therefore the values of c^c must be calculated at each sensor for all potential source locations. This can be accomplished by solving the "forward"-in-time dispersion problem considering as source all potential source locations. However, in the cases examined in this paper the potential source locations are virtually infinite. Therefore, it is computationally more efficient to calculate the c^c 's in an inverse mode, using the concept of the "Source-receptor functions" (SRFs) which describe the sensitivity of concentration at a receptor to the parameters of the emitting source. To this end, the adjoint form of the dispersion model is run using each time as source a sensor location. The differential — steady state — equation of the adjoint variable c^* is:

$$\frac{\partial c_n^*}{\partial t} - u_i \frac{\partial c_n^*}{\partial x_i} - \frac{\partial}{\partial x_i} D \frac{\partial c_n^*}{\partial x_i} = p_n \tag{2}$$

where n is the measurement point counter, p is the probing function (connecting the value at the measurement point with the value at the computational grid node where the variable is originally calculated), D is the coefficient of turbulent diffusion, u_i are the constant-in-time flow velocity components in a Cartesian coordinate system with coordinates $x_i = (x, y, z)$, i = 1–3. As already mentioned, the latter are calculated by a CFD model. In the particular cases described in this paper a RANS model has been used. The values of D have also been calculated by the CFD model using the standard k-ε turbulence closure scheme (Launder and Spalding, 1974). This turbulence model has been used giving reasonable results in several studies of wind flow and pollutant dispersion in complex urban environments (e.g., Trini Castelli et al., 2017).

The nodes of the numerical grid that is used to spatially discretize and solve Eq. (2) constitute the potential source locations. The calculated concentrations that enter cost function (1) are expressed by the SRF as $c^c = q^s\, c^*$, where q^s is an arbitrary source emission rate. Efthimiou et al. (2017) have shown that an arbitrary value for q^s can be used in the case of a stationary source of a passive and non-reactive tracer. With c^c 's calculated through the SRFs, the values of function J (Eq. 1) are calculated for all potential source locations (i.e., at all grid nodes) and their minimum indicates the estimated source location.

Having identified by the above procedure the grid node, k^s, where the source is located, the source emission rate is calculated from the following equation:

$$q^s = \frac{\sum_{n=1}^{K} c_{n,k^s}^* c_n^o}{\sum_{n=1}^{K} \left(c_{n,k^s}^*\right)^2} \tag{3}$$

where K is the number of sensors and c_{n,k^s}^* is the value of the adjoint variable from sensor n at the node k^s.

The method presented above has recently been extended by Kovalets et al. (2018), to deal with problems of transient pollutant dispersion under stationary meteorological fields, allowing for the identification of the location, start time, duration and quantity of emitted substance of an unknown air pollution source of finite time duration.

2. THE WIND TUNNEL EXPERIMENTS

2.1 The MUST wind tunnel experiment

The methodology has been validated against data of the MUST wind tunnel experiment (Bezpalcova and Harms, 2005) which have been scaled up for the conditions of the corresponding field experiment (Yee and Biltoft, 2004). Hence the CFD ADREA-HF code (Efthimiou et al., 2016) has been setup for the simulation in the field scale and all the experimental and computational parameters below are given in the field scale.

In MUST experiment the obstacles were arranged in 12 rows, each consisting of 10 obstacles. The obstacles were nearly identical and had average length, width and height 12.2 m × 2.42 m × 2.54 m respectively. The contaminant's concentration has been measured by a 256-detectors array arranged along obstacle rows in the part of the domain covered by the plume (Fig. 1 in Efthimiou et al., 2017). All detectors were placed at the same height equal to 1.28 m. Non-zero concentrations have been measured by nearly all (244 out of 256) detectors. Here it is noted that only the measurement data that were available to the authors (through data base of COST Action 732) are taken into account.

The wind flow was characterized by neutral stratification, wind speed at the roof level U_{ref} = 8 m/s, (field scale) and wind direction −45° (Fig. 1 in Efthimiou et al., 2017) in the experimental coordinate system.

The contaminant originated from a point source located at the ground level (Fig. 1 in Efthimiou et al., 2017). The volume flow rate of gas at the source was: ≈ 3.3×10^{-6} m^3s^{-1}.

2.2 The "Michelstadt" wind tunnel experiment

The "Michelstadt" wind tunnel experiment represents an idealized Central-European urban environment and has been extensively used in the past for model validation purposes (Efthimiou et al., 2016; Efthimiou et al., 2018*; Baumann-Stanzer et al., 2015). The wind tunnel model had a geometric scale equal to 1:250. Flow and concentration measurements were performed at various locations and heights above ground. There were seven release scenarios corresponding to different point source locations (in open squares, narrow or wide streets, streets aligned perpendicular or parallel to the prevailing large-scale flow, courtyards) and two different incident wind directions (0° and 180°, Fig. 1 in Efthimiou et al., 2018). The reference velocity U_{ref} (at reference height 99.9 m) was equal to 6 ms^{-1}. Only cases with continuous releases of the tracer substance have been considered in the present study. More information about the experiment can be found in www.elizas.eu.

2.3 The Complex Urban Terrain Experiment (CUTE) wind tunnel experiment

The CUTE experiment was carried out to test atmospheric dispersion models with potential use in the wider context of emergency response related to accidental air pollution in urban areas (Baumann-Stanzer et al., 2015). The test site was the downtown area of a typical Central European city. The building heights were between 25 and 35 m. The wind tunnel model had a geometric scale equal to 1:350. The available information for the flow field of the CUTE wind tunnel dataset was limited to the wind speed and direction at a reference height (z_{ref} = 49 m). The wind direction was 235° (south-westerly winds) and the wind speed U (z_{ref}) was equal to 6 m/s. This strategy was adopted to test the dispersion model under realistic emergency conditions, where limited meteorological data would be available (possibly from 1 meteorological station). Therefore, wind velocity measurements were not available. Only tracer concentration data were available for model validation purposes. In the present paper, we used the data collected from "case 3" of the CUTE wind tunnel experiment. In the chosen case, the tracer gas was released at a steady rate from a point source located between houses near the river on the opposite side of the harbour (**Σφάλμα! Το αρχείο προέλευσης της αναφοράς δεν βρέθηκε.** in Efthimiou et al., 2018). The concentration-time series were measured by 34 sensors which locations are shown in **Σφάλμα! Το αρχείο προέλευσης της αναφοράς δεν βρέθηκε.** in Efthimiou et al. (2018).

Besides the continuous release case considered in the present paper, puff release cases were also included in the series of the CUTE experiments. Such cases were considered by Kovalets et al. (2018).

3. RESULTS AND DISCUSSION

In order to quantify the error in locating the source, the horizontal $r_H = \sqrt{\left(x^s - x_t^s\right)^2 + \left(y^s - y_t^s\right)^2}$ and vertical $r_V = \left|z^s - z_t^s\right|$ distances of the estimated source location (x_s, y_s, z_s) from the true source location (x_t^s, y_t^s, z_t^s) have been calculated. Concerning the source rate, the relative source rate ratio $\delta q = \max\left[\left(q^s / q_t^s\right), \left(q_t^s / q^s\right)\right]$ has been calculated which is always greater than unity for both underestimated and overestimated source rates.

The distances between calculated and actual source location and the emission rate ratios that have been obtained are presented in Table . The results of the MUST experiment are very good. For Michelstadt experiment, the method presents variable performance. For the horizontal distance, r_H, a satisfactory performance is obtained for cases S4_0^o, S5_0^o, S6_180^o and S7_180^o, with the best result achieved for the case S5_0^o (r_H = 4.5 m). For the cases S2_0^o, S5_180^o and S8_180^o the horizontal distance between the estimated and the true source location is larger, with the largest obtained for case S8_180° (r_H = 85.50 m). For the vertical distance, r_V, the best performance is achieved for the case S6_180^o (r_V = 1.5 m) while the worst for the case S8_180^o (r_V = 21.5 m). For the source rate ratio, δq, the best performance is achieved for the case S4_0^o and S8_180^o (δq = 1.01) while the worst for the case S2_0^o (δq = 2.25). No systematic dependence can be observed between the number of sensors and the method's accuracy to estimate the source location or strength. So, the performance of the method depends on the characteristics of the source location (open space in the urban area, street canyon perpendicular or parallel to the wind direction, heights of nearest buildings) and the spatial distribution of the sensors in the urban area or in relation to the source. For the CUTE experiment, which is a real urban configuration and therefore more complex than MUST and Michelstadt, the method presents a satisfactory performance which indicates its robustness. The method robustness is also indicated by the fact that in all examined cases the method has converged to a —at least acceptable —solution. It is also worth noting that the inverse source term estimation method does not use any prior information regarding the source characteristics.

Table 1: Horizontal and vertical distances between estimated and true source locations, and relative source rate ratios for the considered test cases.

Test Case	r_H (m)	r_V (m)	δq (-)	Number of sensors
S2_0^o	62.36	9.5	2.25	57
S4_0^o	13.12	17.5	1.01	25
S5_0^o	4.50	3.5	1.05	22
S5_180^o	72.54	11.5	1.65	35
S6_180^o	9.39	1.5	1.97	38
S7_180^o	8.28	13.5	1.14	117
S8_180^o	85.5	21.5	1.01	58
CUTE	13.69	3.97	1.62	34
MUST	1.2	0.1	1.69	244

Each horizontal and vertical distance presented in Table can be divided by the corresponding maximum dimension of the computational domain in the horizontal and vertical directions in order to examine the relative magnitude of the error in the prediction of the source location. The maximum horizontal dimensions of the computational domains for the three experiments were 2094.5 m, 5026.7 m and 361.8 m for Michelstadt, CUTE and MUST, respectively. The vertical dimensions of the computational domains were 144 m, 648 m and 21 m, respectively. The results obtained are presented in Figure . It is clear that in the vertical direction the relative errors in source location are higher than in the horizontal direction. This difference is probably due to that all sensors are located at the same vertical level (near ground). The maximum error in vertical location is equal to 14.93% of the domain height for the S8_180^o case of the Michelstadt experiment. However, the same case presented the best performance for the relative source rate ratio (Table). Also, the best performance for both horizontal and vertical errors is observed for the cases S6_180^o (Michelstadt), CUTE and MUST.

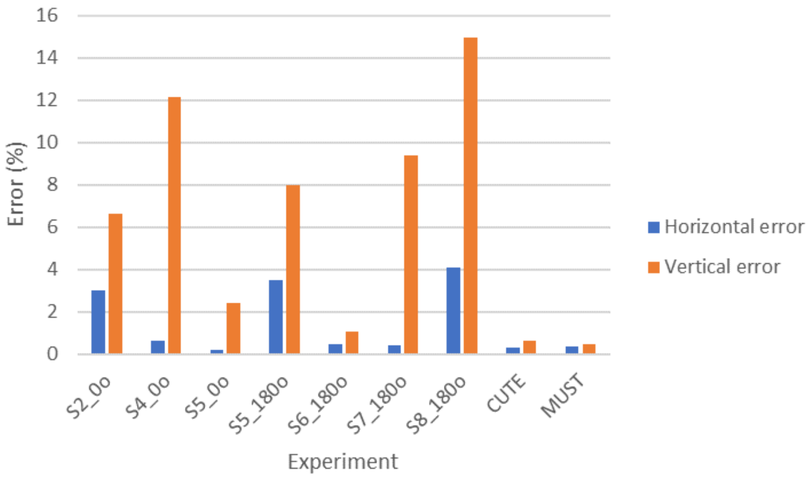

Figure 1. The magnitude of the relative error in the prediction of the source location. Each horizontal and vertical distance presented in Table is divided by the corresponding maximum dimension of the computational domain in the horizontal and vertical direction.

Potential connection of the method's performance with the position of the source was examined. For this reason, two cases have been distinguished: a) the source is located in a street canyon (MUST, S4_0^o, S5_0^o, S5_180^o, S6_180^o, S7_180^o) and b) the source is located in a more open space (S2_0^o, S8_180^o, CUTE). Figure presents the magnitude of the horizontal error against the experiments. There is a tendency of the first group (the street-canyon-located sources) to present smaller errors than the second group (the open-area-located sources).

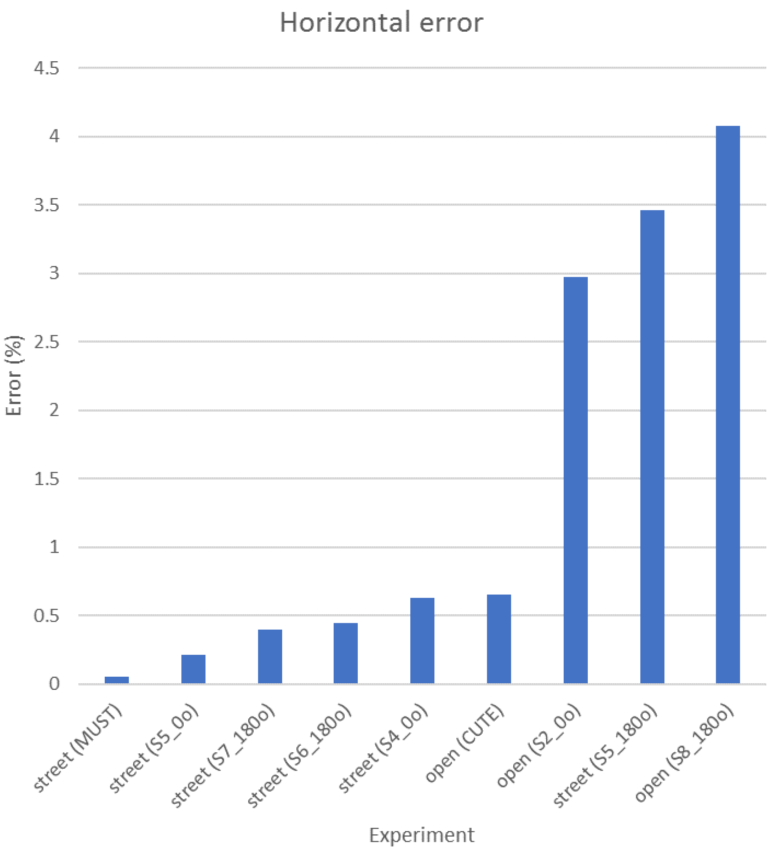

Figure 2. The magnitude of the horizontal relative error of Figure against the two groups of source locations (open-area and street-canyon-located sources).

This can be explained by the fact that the buildings reduce the available space where the source could be located, resulting in a better prediction of the source position. It should be noticed also that the two cases S5_0^o and S5_180^o presented very different performance in locating the source even if it was the same source. This is an indication that the orientation of the street canyon in relation to the incident wind plays also an important role in the performance of the method. Indeed, an additional LES of the Michelstadt experiment (Koutsourakis, 2017) has revealed that due to the perpendicular orientation of the street canyon in relation to the wind direction, a spiral vortex is formed along the street canyon. This increases the uncertainty in locating the source inside the canyon.

4. APPLICABILITY OF THE METHOD FOR EMERGENCY RESPONSE

The above-mentioned works have created to authors further thoughts about their applicability for emergency response. The present authors develop this period a “smart” algorithm for the identification of the point source (location and rate) of airborne materials in complex urban environments. The algorithm selects from a database the appropriate SRFs, according to the incident wind direction and the sensors that detected the hazardous substance, to calculate the cost function, to minimize it and to estimate the location of the source and release rate. The SRF database is constructed during the preparatory phase for various wind directions, wind speeds and stability conditions using the ADREA-HF code. The University of Doha in Qatar was selected as the pilot test case which includes a quite complex configuration of buildings. The algorithm provided robust results in very low execution times (less than 10s) indicating its suitability for emergency response.

The “smart” algorithm that has been developed up to now is a computational system written in FORTRAN language and is presented schematically in Fig. 3. The present version of the algorithm consists of three steps:

1. In the first step the user provides the input data which are: a) the incident wind direction and b) the real concentration values at the sensors (16 fixed sensors for the examined pilot test case).
2. In the second step the algorithm finds the records in the SRF database of one of the wind directions (16 wind directions for the examined pilot test case) in case that the input wind direction coincides with one of them. In case the input wind direction is not the same with one of the wind directions included in the database then the two closest wind directions of the database are sought, and linear interpolation is applied using the corresponding SRFs.
3. Finally, in the third step, according to the incident wind direction and the sensors that detected the hazardous substance the cost function is calculated, it is minimized, and the location of the source and the release rate are estimated (up to now the algorithm was tested for continuous release but it can be further developed for transient releases).

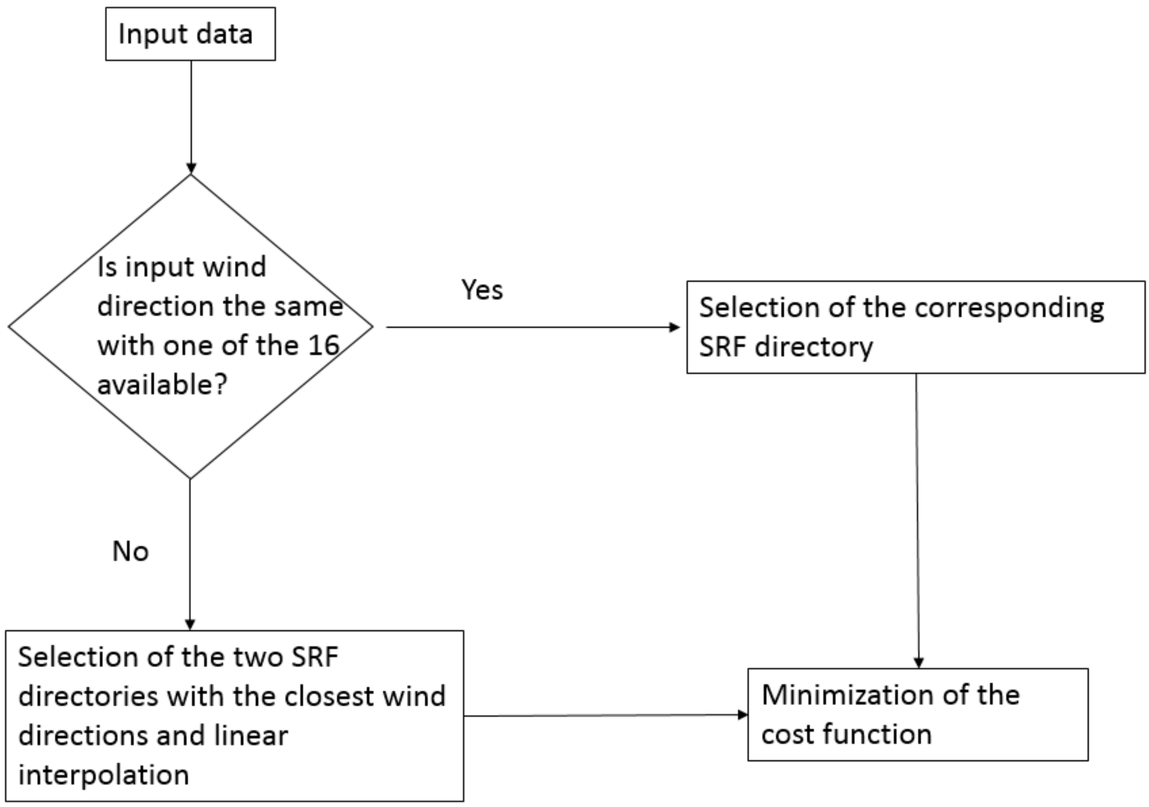

Figure 3. Schematic representation of the "smart" algorithm for the identification of the source.

CONCLUSIONS

The work described herein focuses on the validation of an inverse modelling method for estimating the location and emission rate of an unknown point stationary source of passive atmospheric pollutant in an urban geometry. The cases studied were three wind tunnel experiments, namely MUST, Michelstadt and CUTE. Michelstadt and CUTE represent real (or very close to real) urban configurations, in comparison to the less realistic configuration of the MUST experiment. Michelstadt and CUTE were also more challenging than the MUST experiment because they had less concentration sensors and diverse source locations (open squares, narrow or wide streets, streets aligned perpendicular or parallel to the prevailing large-scale flow, courtyards). The following conclusions can be drawn from the present study:

- The proposed inverse source term estimation method presented a robust behaviour, having converged to a—at least acceptable—solution in all cases, and has resulted in, in most of the cases, a satisfactory determination of the source location (in the vertical and horizontal directions, considering the dimensions of the area of potential source locations and the complexity of the flow situation) and emission rate. The method does not use any prior information regarding the characteristics of the source.
- The performance of the method varies with the examined scenario, even in the same urban geometry, as the simulations of the Michelstadt experiment have revealed. Therefore, the characteristics of the source location are affecting the accuracy of the method, i.e., whether the source is located in a relatively open space inside the urban area, or it is located inside a street canyon that is perpendicular or parallel to the prevailing wind direction, and the heights of the nearest buildings. Based on the results for the Michelstadt experiment, the spatial distribution of the sensors in the urban area and in relation to the source, rather than their number, plays an important role on the accuracy of the source inversion method.

- The error in the horizontal distance varied between 0.05% and 4.1% of the computational domain maximum dimension. The relative source rate ratio varied between 1.01 and 2.25. The vertical distances between estimated and true source locations presented higher errors than the horizontal distances and varied between 0.5% and 14.93% of the computational domain height.
- There appeared to be no correlation between the errors in horizontal distances, vertical distances and release rate.
- The degree of urban complexity is not the factor that most influences the performance of the inverse methodology. Indeed, while the geometry of CUTE is in principle more complex than that of Michelstadt, the source inversion results in case of CUTE were more accurate.

ACKNOWLEDGMENTS

This publication was made possible by a NPRP award [NPRP 7-674-2-252] from the Qatar National Research Fund (a member of The Qatar Foundation). The statements made herein are solely the responsibility of the authors.

The major part of the simulations was performed in the High Performance Research Computing Facilities in Texas A&M University at Qatar. The grid sensitivity analysis of the Michelstadt experiment was supported by computational time granted from the Greek Research & Technology Network (GRNET) in the National HPC facility ARIS (http://hpc.grnet.gr) under project CFD-URB (pr004009).

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