Modification and validation of a method for estimating the location and rate of a point stationary source of passive non-reactive pollutant in an urban environment

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Introduction (I)

- The characterization of an unknown atmospheric pollutant's source following a release is a special case of inverse atmospheric dispersion problem.

- Such kind of inverse problems are to be solved in a variety of application areas such as **emergency response** and **indoor air quality**.

Introduction (II)

- In the urban or industrial scale, few studies have applied **Computational Fluid Dynamics (CFD)** combined with different **source estimation techniques**.

  1. Kumar, P., A.-A. Feiz, S. K. Singh, P. Ngae, and G. Turbelin (**2015**), Reconstruction of an atmospheric tracer source in an urban like environment, J. Geophys. Res. Atmos., 120, 2,589–12,604, doi:10.1002/2015JD024110.
  2. Libre J-M., S. Guérin, A. Castellari, A. Tripathi, M. Leguellec, T. Mailliard and C. Souprayen, **2012**: Source determination in congested environment through Bayesian inference. Int. J. Environment and Pollution, 48, 174–184.
  3. Bady M., S. Kato and H. Huang, **2009**: Identification of pollution sources in urban areas using reverse simulation with reversed time marching method. Journal of Asian Architecture and Building Engineering, 8, 275-282.
  4. Chow F.K., B. Kosovic´ and S. Chan, **2008**: Source inversion for contaminant plume dispersion in urban environments using building-resolving simulations. Journal of applied meteorology and climatology, 47, 1553-1572.
  5. Keats A., E. Yee and F.-S. Lien, **2007**: Bayesian inference for source determination with applications to a complex urban environment. Atmospheric Environment, 41, 465–479.

Introduction (III)

- Kovalets et al. (2011) developed an effective variational algorithm of source inversion combined with an urban-scale CFD model. The performance of the algorithm was evaluated against measurements obtained in MUST wind tunnel experiment and with the Michelstadt wind tunnel dataset.
    - Kovalets I.V., S. Andronopoulos, A. Venetsanos and J.G. Bartzis, 2011: 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.
    - Tsiouri V., I. Kovalets, K.E. Kakosimos, S. Andronopoulos and J.G. Bartzis, 2014: Evaluation of advanced emergency response methodologies to estimate the unknown source characteristics of the hazardous material within urban environments. *HARMO16*, Varna, Bulgaria.
- The medium performance of the algorithm in the second case created second thoughts about the calculation of the source location and rate as well as the effect of various numerical parameters (e.g. grid resolution).

Purpose of the study

- The purpose of the present study is to **modify the cost function** of the source inversion algorithm of Kovalets et al. (2011) for the non-simultaneous calculation of the source location and rate.

- The effects of the grid resolution used for the numerical simulations on the obtained results are also investigated.

Modification of the cost function of the source inversion algorithm (I)

- The cause of the high discrepancy of Tsiouri et al. (2014) between the results and the measurements was the **overfitting** effect.
- **The calculation errors which were introduced by the wrong prediction of the source location and led to significant underestimation of the concentration were compensated by the overestimated source rate.**
- Thus, the resulting quadratic cost function reached minimum for the wrong combined solution (source location and source rate).

$$J = \frac{(x_0^s - x^s)^2}{\sigma_H^2} + \frac{(y_0^s - y^s)^2}{\sigma_H^2} + \frac{(z_0^s - z^s)^2}{\sigma_V^2} + \frac{1}{\sigma_O^2 + \sigma_M^2} \cdot \sum_{n=1}^{K} (c_n^c - c_n^o)^2 \rightarrow \min.$$

Source-receptor function is a function relating concentration at given measurement point to source coordinates and source rate.

$$c_n^c = q_s c_n^*$$

Modification of the cost function of the source inversion algorithm (II)

- A proposed solution to this problem is the separation of source inversion algorithm into the following two steps:
    - Step 1: The source coordinates are analysed;
    - Step 2: Only source rate is analysed.

Modification of the cost function of the source inversion algorithm (III)

- Instead of cost function *J* defined by formula (7) (in Kovalets et al., 2011):

$$J = \frac{(x_0^s - x^s)^2}{\sigma_H^2} + \frac{(y_0^s - y^s)^2}{\sigma_H^2} + \frac{(z_0^s - z^s)^2}{\sigma_V^2} + \frac{1}{\sigma_O^2 + \sigma_M^2} \cdot \sum_{n=1}^{K} (c_n^c - c_n^o)^2 \to \min .$$

a correlation coefficient of measured and calculated concentrations is used:

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

where $\langle \ \rangle$ denotes arithmetic averaging over all measurements while minimum is sought over all possible source locations.

The correlation coefficient is minimized with respect to source coordinates only, while arbitrary source rate, q^s, is used for the minimization procedure.

Modification of the cost function of the source inversion algorithm (V)

- As a second step, the source rate can be identified by minimizing the quadratic cost function with respect to q^s:

$$J = \sum_{n=1}^{K} \left(c_n^c - c_n^o \right)^2 \to \min$$

$$c_n^c = q_s c_n^*$$

Modification of the cost function of the source inversion algorithm (VI)

- The solution of this problem can obviously be obtained analytically by equating to zero the derivative of J with respect to q^s:

$$\frac{\partial J}{\partial q^s} = \sum_{n=1}^{K} \left(q^s c^*_{n,k^s} - c^o_n \right)^2 = \sum_{n=1}^{K} 2c^*_{n,k^s} \left(q^s c^*_{n,k^s} - c^o_n \right) = 0$$

- The solution is obviously:

$$q^s = \frac{\sum_{n=1}^{K} c^*_{n,k^s} c^o_n}{\sum_{n=1}^{K} \left(c^*_{n,k^s} \right)^2}$$

The Complex Urban Terrain Experiment (CUTE) (I)

- The CUTE data set includes results from field and wind tunnel measurements.

- The data set is dedicated to test emergency response tools/atmospheric dispersion models predicting dispersion processes in urban areas (**COST Action ES1006, http://www.elizas.eu/**).

- The second part of the CUTE dataset (CUTE cases 2–4), consists of wind tunnel data.

(source: Environmental Wind Tunnel Laboratory, University of Hamburg)

The Complex Urban Terrain Experiment (CUTE) (II)

- This case corresponds to a real scenario of an accidental release, i.e., only limited information about the boundary conditions is available. For this reason only the wind speed and wind direction at the reference height (6 m/s at 49 m) of the CUTE wind tunnel dataset was available. The wind direction was chosen to be 235 (south-westerly winds).

- The CUTE wind tunnel dataset consists of concentration data only. Concentration time series of tracer gas from continuous releases were measured at pedestrian level. The height of the sensors is 2.1 m.

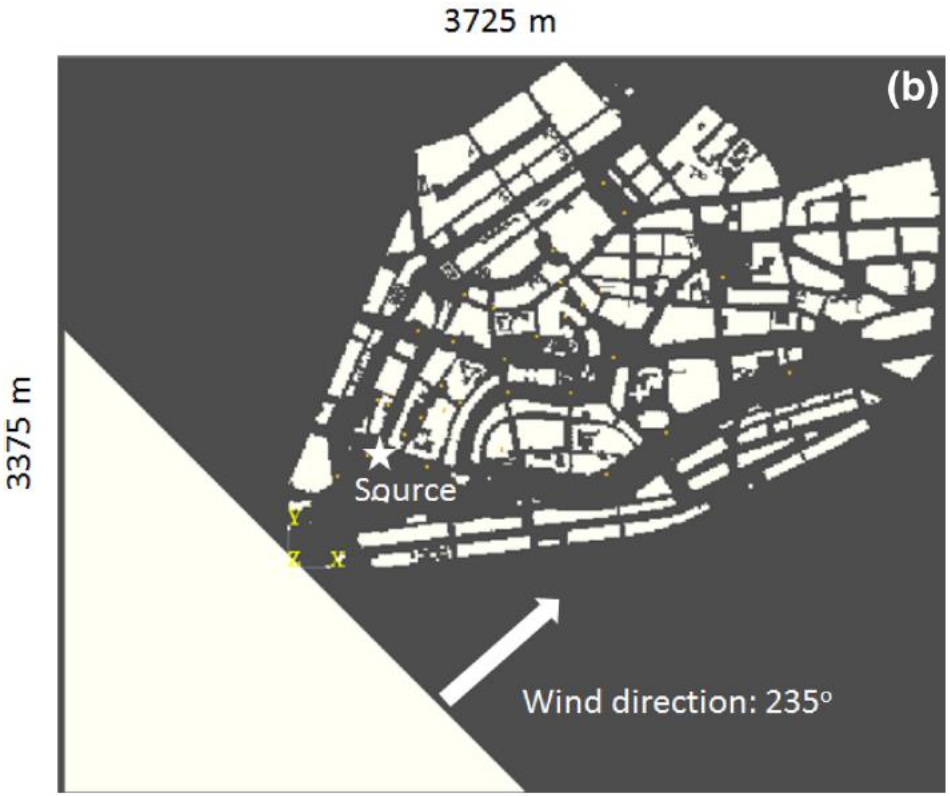
- Concentration measurements are available for three test cases. In each test case the source was placed at a different location. We have selected only one test case 3.

The simulations of the inverse problem (I)

- x = −540 m to 2105.02 m, with the upstream wall of the first obstacle at x = 0 m.

- Domain height of $6H_{max}$ (H_{max} is the maximum bui height equal to 108 m)

- $-540 \text{ m} \leq y \leq 1755.02 \text{ m}$



The simulations of the inverse problem (II)

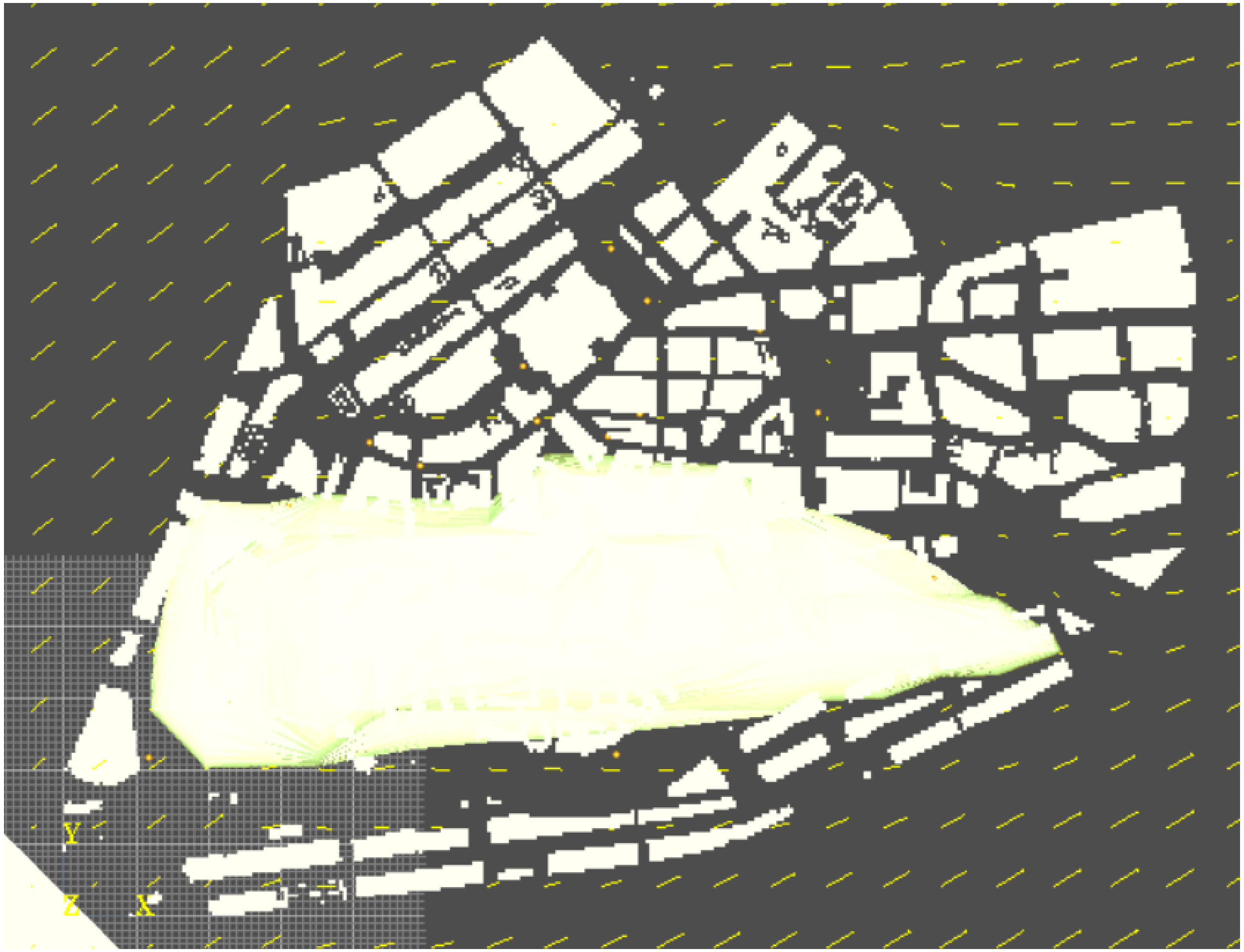
- One coarse and one fine grid have been selected. The number of the control volumes for the coarse grid is 33,000 while for the fine grid is 1,372,800.

- For the coarse grid the minimum cell size in horizontal direction is 78.26 m while for the fine grid it is 9.969 m. Both grids have the same vertical resolution with a minimum cell size close to the ground equal to 1.0 m.

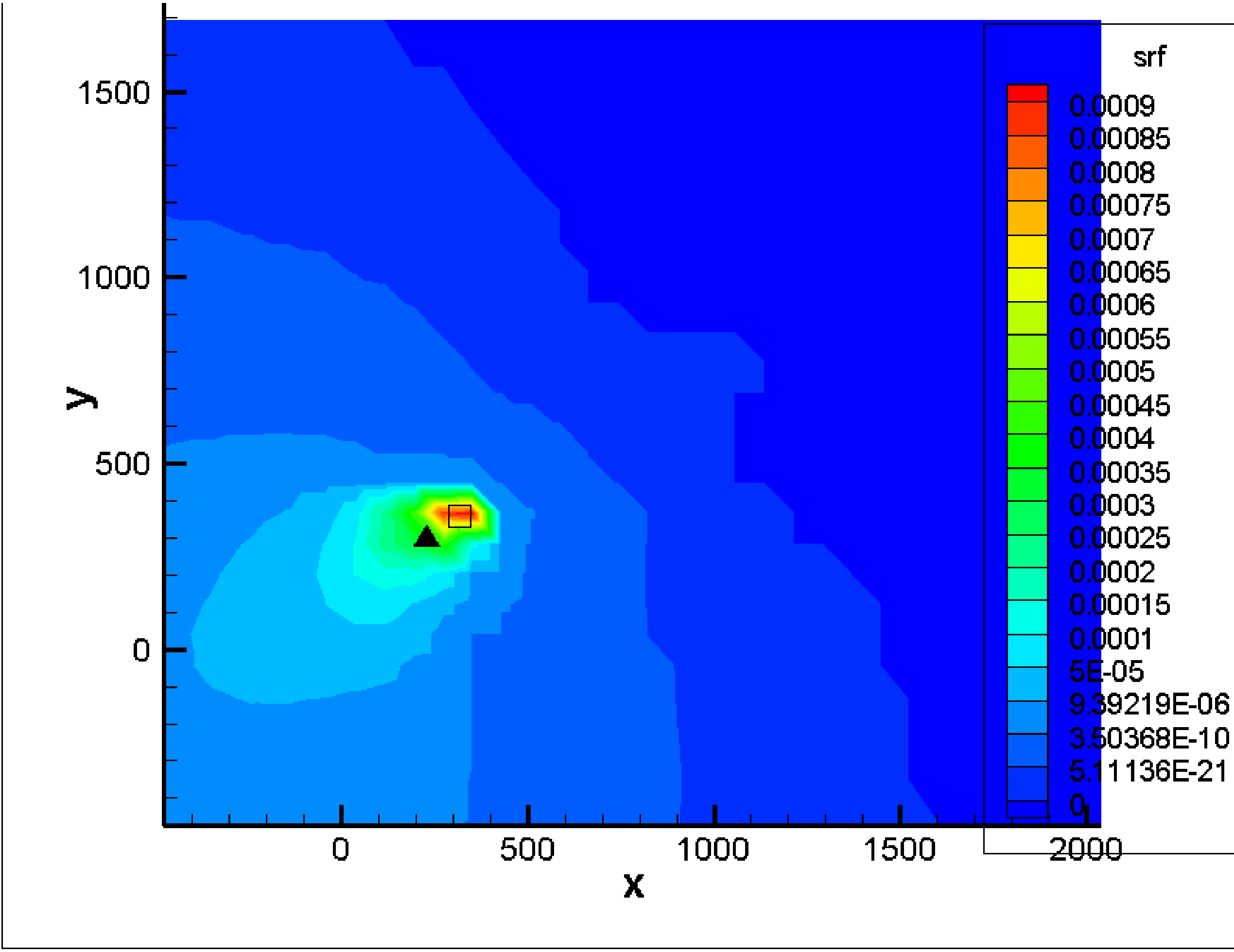
- The boundary conditions of the 3D domain are the same for the forward and the inverse problems. In order to solve the adjoint equation the inverse problem uses the flow results of the forward problem i.e. the mean velocities u, v, w, the turbulent kinetic energy k and the dissipation rate ε.

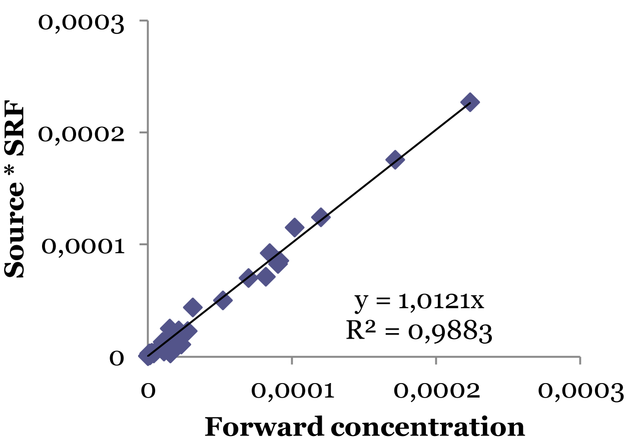
- The non-stationary adjoint equation has been integrated in backward direction through the same time interval as the forward problem (1000 s) to achieve established distributions of adjoint variables. The time step was kept constant and equal to 1 s.

The results of the forward problem



The results of the inverse problem (I)





$$c_n^c = q_s c_n^*$$

The results of the inverse problem (II)

- The performance of the modified algorithm of source estimation was evaluated by three parameters:
  - ▫ Horizontal distance $r_H = \sqrt{\left(x^s - x_t^s\right)^2 + \left(y^s - y_t^s\right)^2}$
  - ▫ Vertical distance $r_V = \left|z^s - z_t^s\right|$

between the estimated and the true source locations.

The results of the inverse problem (III)

- Relative source rate ratio $\delta q = \max\left[\left(q^s / q_t^s\right), \left(q_t^s / q^s\right)\right]$

	Number of cells	r_H (m)	r_V (m)	δq	Solution time
Coarse grid	33,000	77.27	1.55	3.89	16min
Fine grid	**1,372,800**	**0**	**0**	**1.06**	**6h**

Conclusions (I)

- A major change in the data assimilation code included the implementation of a two-step approach:
  - At first only the source coordinates were analysed using a correlation function of measured and calculated concentrations.
  - In the second step, the source rate was identified by minimizing a quadratic cost function.

Conclusions (II)

- The validation of the new algorithm was performed for the source location and rate by simulating a wind tunnel experiment on atmospheric dispersion among buildings of a real urban environment.

- Good results of source location and rate estimation have been achieved when all available measurements (32) were used to solve the inverse problem.

- It was found that the grid resolution plays an important role for the inverse problem.

Future work (I)

1. To decrease the solution time.
   - To perform the simulations in a cluster.

2. To compare our method with other methods.
   - Kumar, P., A.-A. Feiz, S. K. Singh, P. Ngae, and G. Turbelin (2015), Reconstruction of an atmospheric tracer source in an urban like environment, J. Geophys. Res. Atmos., 120, 2,589–12,604, doi:10.1002/2015JD024110.
   - Keats A., E. Yee and F.-S. Lien, 2007: Bayesian inference for source determination with applications to a complex urban environment. Atmospheric Environment, 41, 465–479.

Future work (II)

3. To validate the present methodology with many experiments.
   - MUST wind tunnel by COST Action 732.
   - Michelstadt wind tunnel by COST ES 1006
   - Direct Numerical Simulation by Dr. Omduth Coceal.
   - …

4. To predict the source location and rate in case of puffs.

5. To combine mesoscale with microscale simulations in order to predict the source when it is outside the urban area.

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