Chapter 52
Validation of an Inverse Method for the Source Determination of a Hazardous Airborne Material Released from a Point Source in an Urban Environment

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Abstract An improved inverse method was presented recently for the estimation of the location and the rate of an unknown point stationary source of passive atmospheric pollutant in a complex urban geometry. The inverse method was incorporated in the well-established and updated version of the ADREA-HF Computational Fluid Dynamics code. The key improvement of the proposed inverse method implementation lies in a two-step segregated approach combining a correlation and cost functions. At first only the source coordinates are analyzed 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 new algorithm is performed by simulating the MUST wind tunnel experiment. Overall, we observed significant improvement, compared to previous implementations, on reconstructing the source information (location and rate).

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52.1 Introduction

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 (e.g. Kovalets et al. 2011; Sharan et al. 2012; Singh et al. 2013) pollution control decisions (Koracin et al. 2011) and indoor air quality (Matsuo et al. 2015).

In the urban or industrial scale, there are few researchers that have combined Computational Fluid Dynamics (CFD) with source estimation techniques (Bady et al. 2009; Chow et al. 2008; Keats et al. 2007; Kovalets et al. 2011; Kumar et al. 2016; Libre et al. 2012).

In this point it should be noticed that in some cases of inverse modeling there are some limitations. According to Dhall et al. (2006) there is a typical problem for non-linear least squares fitting due to the ill-posed minimization problem and the non-convex cost function. This problem is called 'overfitting' effect. According to this effect, the calculation errors which are introduced by the wrong source location and lead to significant underestimation of the concentration are compensated by the overestimated source rate. Thus, the resulting quadratic cost function reaches minimum for the wrong combined solution (source location and source rate). In context of data assimilation this problem is especially important when the number of measurements is insufficiently small. This 'overfitting' effect was also observed in Tsiouri et al. (2014) where the Source Inversion (SI) algorithm produced unsatisfactory results regarding the distance between the true and the estimated source location and the true to estimated source rate ratio.

Efthimiou et al. (2016) presented an integrated and innovative approach, to eliminate the 'overfitting' effect, based on two main improvements. First, we propose a non-simultaneous determination of the source location and rate, based on a two-step segregated approach combining a correlation and cost functions. Second, we suggest a correlation coefficient of measured and calculated concentrations, instead of a cost function (as in Kovalets et al. 2011). Moreover, we investigate the impact of the grid resolution, for the numerical simulations, on the determination of source characteristics. The MUST dataset has been selected for the evaluation of the proposed approach owes to its high quality data and because it has been used extensively by other similar works.

A description of the experiment and the computational simulations can be found in Kovalets et al. (2011). The present grid is slightly different than the one of Kovalets et al. (2011). It consists of 58,500 cells with minimum/maximum cell distances $dx = 4.93/9.9$, $dy = 4.95/6.2$ and $dz = 0.2/2.06$.

52.2 Method of Validation of the Predicted Source Location and Rate

In order to understand the order of magnitude of the error we have used the horizontal $r_H = \sqrt{(x^s - x_t^s)^2 + (y^s - y_t^s)^2}$ and vertical $r_V = |z^s - z_t^s|$ 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) where index "t" stays for the true source. We have assumed that the predicted source (x^s, y^s, z^s) is located at the center of the cell.

Concerning the source rate we have calculated the relative source rate ratio $\delta q = \max\left[\left(q^s/q_t^s\right), \left(q_t^s/q^s\right)\right]$ which is always greater than unity for both underestimated and overestimated source rates.

52.3 Computational System

The solution was performed in a Laptop with 8 GB RAM using the OpenMP protocol and all the cores (four) of the processor (Intel(R) Core(TM) i7-4700MQ CPU @ 2.40 GHz).

52.4 Results

The horizontal distance (r_H) between the real and the predicted source was found equal to 10.81 m and the vertical distance (r_V) equal to 0.54 m which are slightly better results than Kovalets et al. (2011) (r_H = 11 m and r_V = 0.8 m).

The relative source rate ratio was found equal to 2.26 which is again better result than Kovalets et al. (2011) (δq = 3.1).

52.5 Conclusions

A major change in the data assimilation code of Kovalets et al. (2011) was performed in Efthimiou et al. (2016) and included the implementation of a two-step approach:

- At first only the source coordinates were analyzed using a correlation function of measured and calculated concentrations.
- In the second step, the source rate was identified by minimizing a quadratic cost function.

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 (244) were used to solve the inverse problem.

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References

Bady M, Kato S, Huang H (2009) Identification of pollution sources in urban areas using reverse simulation with reversed time marching method. J Asian Arch Build Eng 8:275–282

Chow FK, Kosovic´ B, Chan S (2008) Source inversion for contaminant plume dispersion in urban environments using building-resolving simulations. J Appl Meteorol Climatol 47:1553–1572

Dhall JM, Lewis S, Lakshmivarahan SD (2006) Dynamic data assimilation: a least squares approach. Cambridge University Press, p 655

Efthimiou GC, Andronopoulos S, Venetsanos A, Kovalets IV, Kakosimos K, Argyropoulos CD (2016) Modification and validation of a method for estimating the location of a point stationary source of passive non-reactive pollutant in an urban environment. In: 17th international conference on harmonisation within atmospheric dispersion modelling for regulatory purposes, 9–12 May. Budapest, Hungary

Keats A, Yee E, Lien F-S (2007) Bayesian inference for source determination with applications to a complex urban environment. Atmos Environ 41:465–479

Koracin D, Vellore R, Lowenthal DH, Watson JG, Koracin J, McCord T, DuBois DW, Chen L-WA, Kumar N, Knipping EM, Wheeler NJM, Craig K, Reid S (2011) Regional source identification using Lagrangian stochastic particle dispersion and HYSPLIT backward-trajectory models. J Air Waste Manag Assoc 61:660–672

Kovalets IV, Andronopoulos S, Venetsanos A, Bartzis JG (2011) Identification of strength and location of stationary point source of atmospheric pollutant in urban conditions using computational fluid dynamics model. Math Comput Simul 82:244–257

Kumar P, Singh SK, Feiz A-A, Ngae P (2016) An urban scale inverse modelling for retrieving unknown elevated emissions with building-resolving simulations. Atmos Environ 140: 135–146

Libre J-M, Guérin S, Castellari A, Tripathi A, Leguellec M, Mailliard T, Souprayen C (2012) Source determination in congested environment through Bayesian inference. Int J Environ Pollut 48:174–184

Matsuo T, Kondo A, Shimadera H, Kyuno T, Inoue Y (2015) Estimation of indoor contamination source location by using variational continuous assimilation method. Build Simul 8:443–452

Sharan M, Singh SK, Issartel JP (2012) Least square data assimilation for identification of the point source emissions. Pure Appl Geophys 169:483–497

Singh SK, Sharan M, Issartel JP (2013) Inverse modelling for identification of multiple-point releases from atmospheric concentration measurements. Bound Layer Meteorol 146:277–295

Tsiouri V, Kovalets I, Kakosimos KE, Andronopoulos S, Bartzis JG (2014) Evaluation of advanced emergency response methodologies to estimate the unknown source characteristics of the hazardous material within urban environments. HARMO16, Varna, Bulgaria