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An optimized inverse modelling method for determining the location and strength of a point source releasing airborne material in urban environment

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HIGHLIGHTS

- Improved inverse source term identification method: source location and emission rate.
- Variational, 2-steps method: (1) source coordinates (2) emission rate estimation.
- Method incorporated in computational fluid dynamics code applicable in urban areas.
- Successful validation through simulation of MUST wind tunnel experiment.
- Performance of the method evaluated depending on size of measurement stations network.

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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 is incorporated in the Computational Fluid Dynamics code ADREA-HF and presented in this paper. The key improvement in relation to the previous version of the method 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 new algorithm is performed by simulating the MUST wind tunnel experiment. A grid-independent flow field solution is firstly attained by applying successive refinements of the computational mesh and the final wind flow is validated against the measurements quantitatively and qualitatively. The old and new versions of the source term estimation method are tested on a coarse and a fine mesh. The new method appeared to be more robust, giving satisfactory estimations of source location and emission rate on both grids. The performance of the old version of the method varied between failure and success and appeared to be sensitive to the selection of model error magnitude that needs to be inserted in its quadratic cost function. The performance of the method depends also on the number and the placement of sensors constituting the measurement network. Of significant interest for the practical application of the method in urban settings is the number of concentration sensors required to obtain a "satisfactory" determination of the source. The probability of obtaining a satisfactory solution – according to specified criteria –by the new method has been assessed as function of the number of sensors that constitute the measurement network.

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1. Introduction

The characterization of an unknown atmospheric pollutant's source (i.e., assessment of its location and emission rate) following

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a release (i.e., using the available observations) is a special case of inverse atmospheric dispersion problem. The inverse dispersion problems are solved by combining in some optimal way results of computational dispersion models and existing measurements. 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; Ben Salem et al., 2016) pollution control decisions (Koracin et al., 2011), indoor air quality (Matsuo et al., 2015) and monitor of nuclear testing (Pudykiewicz, 1998). A review of source term estimation methods for atmospheric dispersion events is given in Hutchinson et al. (2017).

In the urban or industrial plant spatial scale, where complex and turbulent meteorological conditions arise due to the interaction of the air flow with the buildings, there are few researchers that have combined Computational Fluid Dynamics (CFD) with source estimation techniques (Mons et al., 2017; Xue et al., 2017a, 2017b; Kumar et al., 2016; Kumar et al., 2015; Libre et al., 2012; Kovalets et al., 2011; Bady et al., 2009; Chow et al., 2008; Keats et al., 2007). In Mons et al. (2017) a non-intrusive ensemble-based variational data assimilation scheme enhanced by proper orthogonal decomposition was deployed in conjunction with a Large Eddy Simulation (LES) solver. Their methodology was proved to be able to accurately identify both pollutant source and wind characteristics with a computational cost of $O(10)$ LES simulations. In Xue et al. (2017a) the Bayesian inference was used to improve estimation accuracy by treating the Schmidt number as an extra unknown parameter. A wind tunnel experiment with a constant point tracer source in an urban-like geometry was used. The results showed that Schmidt had a major impact on estimation. Larger Schmidt values shifted the estimated location towards the upwind direction and decreased the estimated strength. The same authors (Xue et al., 2017b) used a two-step deterministic approach for identifying the point source with a constant emission rate in built-up urban areas. The analytic form of the marginal posterior probability density function of the source location was derived to estimate the source location. The emission rate was then estimated using the conditional posterior distribution. Their method was tested using data obtained in two wind tunnel scenarios of contaminant dispersion in typical urban geometries represented by block arrays. CFD modelling and the adjoint equations were used to calculate the building-resolving source-receptor relationship required in the identification. In Kumar et al. (2016) a source inversion methodology was based on the renormalization inversion theory coupled with a building resolving CFD (i.e. fluidyn-PANACHE) modelling approach which estimates the release height along with the projected location on the ground surface and the intensity of an unknown continuous point source in an urban area. In Kumar et al. (2015) a methodology was described combining a renormalization inversion technique with a building-resolving CFD approach for source retrieval in the geometrically complex urban regions. The renormalization inversion approach was based on an adjoint source-receptor relationship. Libre et al. (2012) CFD (i.e. Fluidyn-PANEPR) was used to model the dispersion while the Bayesian inference algorithm enabled the estimation of the source term in real time. The modelling platform based on these developments produces real time 3D concentration fields owing to precalculated wind fields patterns selected from a database on the basis of real time meteorological data acquisition. Bady et al. (2009) examined the accuracy of the inverse CFD (Star-CD) modelling in a simple laminar flow, but focused on the source location. The pollutant was emitted for variable wind conditions and the wind flow around a single building was investigated for two different sources. In both cases the numerical concentration results of the forward problem were used as concentration measurements for the inverse problem. By using the peak concentration as indicator, they could identify the source of the pollution. Chow et al. (2008) used Bayesian inference via stochastic sampling algorithms with a high-resolution CFD code (FEM3MP) in order to reconstruct an atmospheric release event and to determine the plume source and release rate based on point measurements of concentration. The CFD model has been used as a 'black-box', i.e., for each set of input parameters the model was run in forward mode to obtain the corresponding set of output parameters. In Keats et al. (2007) a similar probabilistic formulation of inverse problem was adopted and posterior distribution function was evaluated with Monte-Carlo sampling. However instead of using a CFD model (i.e. urbanSTREAM) as a 'black box' tool, a 'source-receptor' function was constructed using the adjoint transport equation, as per Marchuk (1982) and Marchuk (1996).

At this point it should be noted that there are limitations in some cases of inverse modelling. 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 a wrong source location estimation are compensated by error in estimated 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 small. For example, in Kovalets et al. (2009) the cost function was minimised with respect to both wind field and source rate. It was found that for too coarse resolution of the monitoring network the Normalized Mean Squared Error of the concentration field (closely related to the value of cost function) decreased in the data assimilation process while the error of the wind field (being part of the solution vector) increased. This 'overfitting' effect was also observed in the work of Tsiouri et al. (2014) in which 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.

This study presents an integrated and innovative approach, to eliminate the 'overfitting' effect, based on the following improvement: a non-simultaneous determination of the source location and rate is proposed, based on a two-step segregated approach that combines a correlation coefficient and a cost function, instead of using a single cost function as was done by Kovalets et al. (2011). The correlation coefficient of measured and calculated concentrations is used to estimate the source location, while the quadratic cost function is directly solved to calculate the emission rate. In the following part of the paper, the new version of the method is described in detail and then both old and new versions are intercompared by applying them on the MUST wind-tunnel experimental dataset. This experiment has been selected because of its high quality data and its extensive use in other similar works. The source term estimation method is based on the calculated flow field, so a grid independent solution for the wind flow field is firstly obtained by applying successive refinements of the computational mesh. However, the old and new source term estimation methods are tested on both coarse and fine grids, to assess their dependence on the grid resolution, in combination to other parameters. In the last part of the paper the dependence of the new method's performance on the number of measuring sensors is examined.

2. Methodology

In general, solving the inverse atmospheric dispersion problem consists of estimating the posterior joint probability distribution of the unknown model parameters (usually the source spatial coordinates and emission rate), the measurements and the prior

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