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Inverse identification of unknown finite-duration air pollutant release from a point source in urban environment

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ABSTRACT

In this work, we present an inverse computational method for the identification of the location, start time, duration and quantity of emitted substance of an unknown air pollution source of finite time duration in an urban environment. We considered a problem of transient pollutant dispersion under stationary meteorological fields, which is a reasonable assumption for the assimilation of available concentration measurements within 1 h from the start of an incident. We optimized the calculation of the source-receptor function by developing a method which requires integrating as many backward adjoint equations as the available measurement stations. This resulted in high numerical efficiency of the method. The source parameters are computed by maximizing the correlation function of the simulated and observed concentrations. The method has been integrated into the CFD code ADREA-HF and it has been tested successfully by performing a series of source inversion runs using the data of 200 individual realizations of puff releases, previously generated in a wind tunnel experiment.

1. Introduction

The source inversion problem - identification of the unknown source properties such as location, release rate, and others, following the detection a plume by a monitoring network - is of great practical interest (Hutchinson et al., 2017). This problem (also called source term estimation) becomes even more important when hazardous toxic pollutants are detected in cities following accidental or deliberate releases, because the large density of urban population increases its vulnerability to such events. From one side, the complex nature of atmospheric transport processes in urban atmospheric environment could be treated most comprehensively by Computational Fluid Dynamics (CFD) models (Fisher et al., 2010). From the other such models are usually time-consuming, and so, their usage in real-time emergency response systems is challenging (e.g. Kovalets et al., 2008; Moussafir et al., 2014).

The issue of the real-time applicability is even more pronounced in case of source inversion problems. Their solution often requires multiple runs of the atmospheric dispersion model (ADM) especially when combined with Bayesian inference or ensemble Kalman filtering techniques (Bieringer et al., 2017; Van Velzen and Segers, 2010; Osorio Murillo et al., 2015). Hence simplified Gaussian plume and Gaussian puff models are frequently used to solve source inversion problems (e.g., Schauberger et al., 2013; Brambilla and Brown, 2013; Petrozziello et al., 2017; Hutchinson et al., 2017; Salem et al., 2017). In case of application of CFD models for source term estimation the number of model integrations could be reduced with the aid of the so-called source-receptor function (SRF). SRF is the relationship that is used instead of the forward model integration, together with various parameters of the source term. The SRF is calculated using backward adjoint equations (Marchuk, 1996, Pudykiewicz, 1998). This approach leads to great reduction in the computational cost of the source inversion.

Several studies reconstructed source parameters by calculating SRFs using backward adjoint equations and combining a CFD model with concentration measurements, in cases of a stationary release of atmospheric pollutant in an urban environment under stationary meteorological conditions (Yee et al., 2008; Keats et al., 2010; Kovalets et al., 2011; Kumar et al., 2015, 2016; Xue et al., 2017; Efthimiou et al., 2017a). The calculation of SRF for the stationary dispersion problem requires $K = N_o$ integrations of backward adjoint equations, with N_o being the total number of measurement stations. In case of transient

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dispersion problem, the necessary amount of computations for calculating the SRF increases dramatically, since it requires as many integrations of backward adjoint equations as the available measurements: $K = \sum_{i=1}^{N_o} M_i$, here M_i is the number of measurements reported by the i-th station. Therefore the required computational time for the SRF calculation increases significantly in the case of a transient dispersion problem as compared to the stationary case.

An interesting practical case of the transient dispersion problem is when the time variation of concentration fields is caused only by the transient release (i.e., finite-duration source emitting in stationary meteorological conditions). As it will be shown below the required time for SRF calculations could be largely reduced in such cases. We consider atmospheric dispersion problems characterized by small enough time intervals (< 1 h) and spatial scales up to about 10 km from the release location for which the assumption of stationary meteorological fields is frequently applied in practice (e.g. Seaman, 2000). Another issue that arises in case of identification of transient releases is that, in addition to source location and release rate which are the only unknowns for stationary release, the onset and duration of the release are also unknown while the release rate is variable. Thus the number of possible source configurations increases and it becomes much more difficult to solve the source inversion problem. The problem is simplified in cases of short duration releases (~1 min) when the release rate can be assumed constant.

Very few studies (e.g., Vervecken, 2015) have considered a source identification problem in case of transient releases in urban atmospheric environments with the application of CFD models. However, in the abovementioned study simplifications were adopted, such as a limited number of known possible source positions. Therefore the goal of the research presented in this paper was to develop a source inversion algorithm in the framework of a CFD ADM, allowing the assessment of the unknown source parameters for short duration releases in an urban environment under stationary meteorological conditions. The proposed algorithm is also capable of handling applications in real-time emergency response systems.

Even under stationary meteorological fields, 'inherently transient features of the flow field' (Blocken et al., 2011) are always present and in reality influence turbulent concentration signals. In the present paper, we use an ADM based on Reynolds-Averaged Navier Stokes (RANS) equations therefore it is not possible to reproduce these features. In this respect we validated the developed approach by performing a series of source inversion runs using data from 200 individual realizations of puff releases that were carried out under the same average flow conditions in the wind tunnel Complex Urban Test Experiment (CUTE) on atmospheric dispersion in urban environment (Baumann-Stanzer et al., 2015). Concentrations were observed to vary significantly between those individual realizations of puff releases due to turbulent nature of the flow (Efthimiou et al., 2017b). Even though we use a RANS ADM the robustness of the developed source inversion approach following assimilation of the variable between puffs concentration measurements is demonstrated.

The present work is a continuation of the previous works by Kovalets et al. (2011), Efthimiou et al. (2016), Efthimiou et al. (2017a), Argyropoulos et al. (2018) in which a stationary release rate was considered. Efthimiou et al. (2017a) proposed to use a correlation-based cost function instead of a "standard" quadratic cost function and confirmed the effectiveness of this approach. As it was demonstrated by Argyropoulos et al. (2018) a correlation-based cost function is also very convenient tool for assimilation of non-standard observations, such as health symptoms. In the present work the source inversion algorithm is extended for the case of finite-duration release and is implemented in the CFD code ADREA-HF (Venetsanos et al., 2010). The mathematical formulation of the proposed algorithm and the testing results from applying it in the CUTE experiment are presented and discussed in the remainder of this paper.

2. Method description

2.1. Statement of source inversion problem

In this work, the source inversion method presented by Kovalets et al. (2011) for a stationary dispersion problem is extended to the case of a transient pollutant release. We consider the advection-diffusion equation of a passive conservative contaminant originating from a point source:

$$\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} - \frac{\partial}{\partial x_i} D \frac{\partial c}{\partial x_i} = q(t)\delta_\varepsilon(x - x^s)\delta_\varepsilon(y - y^s)\delta_\varepsilon(z - z^s) = f^s(x, y, z, t), \tag{1}$$

where c is the Reynolds averaged concentration, D is the coefficient of turbulent diffusion, u_i are the Reynolds-averaged and fixed in time velocity components in a Cartesian coordinate system with coordinates $\bar{r} = (x_1, x_2, x_3) = (x, y, z)$. The solution of Eq. (1) is considered in spatiotemporal domain$G = [0, T] \times \Omega$, where T is the integration time. The right-hand side f^s, in Eq. (1) describes the finite-duration point source located at (x^s, y^s, z^s) and having source rate q^s[kg/s], beginning at time $t = t^s$ and ending at time $t = t^s + \Delta^s$, where Δ^s is the release duration:

$$q(t) = \begin{cases} q^s, & t \in [t^s, t^s + \Delta^s] \\ 0, & t \notin [t^s, t^s + \Delta^s] \end{cases}. \tag{2}$$

The function of scalar argument $\delta_\varepsilon(.)$ in Eq. (1) is a stepwise function:

$$\delta_\varepsilon(\tau) = \begin{cases} 1/\varepsilon, & |\tau| \le \varepsilon \\ 0, & |\tau| > \varepsilon \end{cases}. \tag{3}$$

Here the parameter ε is sufficiently small (much smaller than the spatial scale of the considered atmospheric dispersion problem) so that from a physical point of view the source could be considered as point and as result, the obtained solution does not depend on ε (Vladimirov, 2002). We do not use the Dirac delta function because even though Eq. (1) with Dirac delta function in r.h.s has a solution in the space of generalized functions, the scalar product is not defined in this space, and thus the presentation of the adjoint formalism will not be mathematically correct. From the definition of δ_ε it apparently follows that $\int_0^T dt \int_\Omega f^s \cdot d\Omega = q^s \Delta^s$, where the integration is performed over the spatial domain Ω in which Eq. (1) is considered and $d\Omega$[m^3] is the infinitesimal volume.

Eq. (1) is complemented with initial conditions: $c(x, y, z, 0) = 0$ and with boundary conditions corresponding to zero-fluxes through boundaries:

$$\partial c/\partial \bar{n} = 0, \quad (x, y, z) \in \partial\Omega. \tag{4}$$

Here $\partial\Omega$ is the boundary of the spatial domain, and $\bar{n}$ is the normal vector to it.

Now assume that the measurements are performed by stations located at measurement points with coordinates $\bar{r}_n^o = (x_n^o, y_n^o, z_n^o)$: $1 \le n \le N_o$, N_o being the total number of measurement points. At each station n there are $M(n)$ different concentration measurements $c_{n,m}^o$ performed at different times $t_{n,m}$, where m is the time-index and therefore $1 \le m \le M(n)$. Then the total number of measurements is $K = \sum_{n=1}^{N_o} M(n)$.

Then the problem of estimating the source emission rate and location could be posed as the problem of finding such values of source parameters $x^s, y^s, z^s, t^s, \Delta^s, q^s$ combined in a vector of control parameters $\psi = (x^s, y^s, z^s, t^s, \Delta^s, q^s)^T$, which minimizes the following cost function:

$$J = -\frac{\langle (c^o - \langle c^o \rangle)(c^c - \langle c^c \rangle) \rangle}{\sqrt{\langle (c^c - \langle c^c \rangle)^2 \rangle}\sqrt{\langle (c^o - \langle c^o \rangle)^2 \rangle}} \underset{\psi}{\rightarrow} \min. \tag{5}$$