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SOURCE RECONSTRUCTION IN URBAN AND NON-URBAN ENVIRONMENTS USING AN INVERSION METHODOLOGY COUPLED WITH A CFD APPROACH

Pramod Kumar[1], Amir-Ali Feiz[1], Sarvesh Kumar Singh[1], Pierre Ngae[1], Raj Rani[1], Emerson Barbosa[1], Grégory Turbelin[1], Jean-Pierre Issartel[2], Nadir Bekka[1]

[1]LMEE, Université d'Evry-Val d'Essonne, 40 Rue du Pelvoux, 91020 Evry, France
[2]NRBC, Centre d'Etudes du Bouchet, 5 Rue Lavoisier, BP 3, 91710 Vert le Petit, France

Abstract: Accurate and fast reconstruction of the atmospheric pollutant sources in urban and non-urban regions is essential for emergency regulators to detect the unknown accidental or deliberated releases. This study describes a methodology combining a recently proposed renormalization inversion technique with a building-resolving Computational Fluid Dynamics (CFD) approach for source retrieval in the non-urban and geometrically complex urban regions. The source parameters (i.e. source location, height, and release rate) are reconstructed from a finite set of point measurements of concentration acquired from some sensors and the adjoint functions computed from a CFD model *fluidyn*-PANACHE. Two different experimental datasets (i) Fusion Field Trial-2007 (FFT-07) in flat terrain and (ii) Mock Urban Setting Test (MUST) field experiment in real situations at an urban scale are used for evaluation of the methodology. For both tracer experiments, the inversion results are presented with both synthetic and real measurements in various atmospheric stability conditions. The source locations were retrieved close to their true release locations at urban scale in MUST field experiment and FFT-07 in flat terrain with the real measurements. The study highlights the effectiveness and detection feasibility of the renormalization inversion technique coupled with a CFD modeling system to estimate the unknown source parameters in urban and non-urban regions.

***Key words:** CFD modeling, Inverse problem, FFT-07, MUST field experiment, Renormalization inversion theory*

INTRODUCTION

Fast and accurate identification of an unknown atmospheric tracer source in urban and non-urban regions can reduce the extent of subsequent exposure and associated mortality of an accidental or deliberated incident. The source reconstruction provides information about number of sources, their locations, height, and emission rates. A source reconstruction process generally utilizes the concentration measurements of a pollutant observed by a finite number of detectors distributed over a region. However, these concentration measurements, detected over a threshold value of a sensor, alone provide no particular information about the source including its location and release rate. An inversion methodology is required to estimate an unknown contaminant source based on these limited concentration measurements.

Several inversion procedures are described in the literature and recently, Issartel et al. (2007) proposed the renormalization inversion technique for identification of a distributed source in a region. The renormalization inversion technique required the computation of the adjoint functions corresponding to each concentration measurement. Recently, Sharan et al. (2009) extended the renormalization inversion technique to identify a continuous point release. This technique was applied and evaluated to retrieve a point source in flat and homogeneous terrains, where the consideration of a constant flow-field throughout a region is sufficient to compute the adjoint functions by a simple Gaussian model. However, flow-field throughout a complex urban region is generally not constant and diverted into often unexpected directions by the presence of buildings and other obstacles. In a recent study, Kumar et al. (2015) described a methodology based on the renormalization inversion technique and a building-resolving computational fluid dynamics (CFD) approach for reconstruction a continuous point source in the geometrically complex urban regions. The methodology was evaluated with 20 trials from Mock Urban Setting Test (MUST) field experiment in various atmospheric stability conditions. However, the methodology was described and evaluated in a two-dimensional space to retrieve a ground-level source or the emission sources along a horizontal cross-section area passing through a fixed vertical level. The problem of vertical structure in continuous atmospheric source reconstruction in an urban area in 3-dimensional space is not described. This study addressed this problem of vertical structure in atmospheric source reconstruction. The objective of this study is to estimate the release height, location, and strength of a source in the urban and non-urban regions in 3-dimensional space.

METHDOLOGY AND MODEL

An inversion technique, based on a concept of the renormalization theory (Issartel et al., 2007; Sharan et al., 2009), is utilized here for reconstruction of a continuous point source in 3-dimensional (3-D) space. It estimates the source parameters, *viz.* location, height, and intensity of a point release. The renormalization inversion technique returns an emission estimate linear with respect to a finite number m of concentrations measurements $\boldsymbol{\mu}$. It required to compute the adjoint functions $a_i(\mathbf{x})$, also known as retroplumes, in a 3-dimensional computational domain $\mathbf{x} = (x, y, z)$, corresponding to each concentration measurement at the receptor. The renormalization technique utilises these retroplumes to compute the renormalized weight functions $w(\mathbf{x})$ in a 3-dimensional domain, and then these weight functions $w(\mathbf{x})$ along with the concentration measurements $\boldsymbol{\mu}$ compute a source estimate function $\mathbf{s}(\mathbf{x})$. In a case of point release, the maximum value of the source estimate function $\mathbf{s}(\mathbf{x})$ coincides with a position $\mathbf{x}_0 = (x_0, y_0, z_0)$ of a point source. Once the location $\mathbf{x}_0$ is identified in a 3-D domain, the intensity q_0 of the estimated point source is computed by $q_0 = \mathbf{s}(\mathbf{x_0})\, w(\mathbf{x_0})^{-1}$. A detailed mathematical description of the renormalization theory for a continuous point source retrieval in 2-D space and various issues and limitations are given in Sharan et al. (2009). However, the inversion methodology is implemented and evaluated here to address the problem of vertical structure in the atmospheric source reconstruction in 3-dimensional domain.

An important step of the inversion technique for source reconstruction is accurately computations of the adjoint functions in urban or non-urban environments. Computation of the adjoint functions by a dispersion or adjoint model required the realistic flow-field in the urban environments. The flow-field in urban regions is complex because the buildings and other obstacles often diverted it into unexpected directions. The CFD models has shown their applicability for computations of the realistic flow-field in urban regions and can be useful to compute the representative adjoint functions. Consideration of the constant flow-field throughout a domain in flat or non-urban terrains is often solve the purpose to compute the adjoint function by a simple Gaussian model. However, recent studies shows that the CFD models can also provide a more realistic flow and dispersion phenomena in homogeneous flat terrains in various atmospheric stability conditions.

This study utilises a CFD model *fluidyn*-PANACHE® to compute the flow-field and adjoint functions in urban and non-urban terrains. The *fluidyn*-PANACHE is a 3-dimensional Computational Fluid Dynamics (CFD) diagnostic model for simulating atmospheric processes related to the pollution and hazard in complex geometric environment. It solves the Reynolds Average Navier Stocks (RANS) equation governing air motion using 3-D finite-volume techniques and includes a built-in automatic 3-D mesh generator that can create the finite-volume mesh around obstacles and body-fitting the terrain undulations. To resolve the turbulent structure in computational domain, it includes a modified standard k-ϵ 3-D prognostic turbulence model. Dispersion of a tracer in the atmosphere is described by the advection-diffusion equation in Eulerian framework in *fluidyn*-PANACHE. To compute the retroplumes at each receptor, the flow-field is reversed by 180° and transport equation is integrated backward in time.

TRACER FIELD EXPERIMENTS

The source reconstruction methodology coupled with a CFD approach is evaluated with two tracer field experiments, namely, Fusion Field Trial 2007 (FFT-07) experiment in flat terrain and Mock Urban Setting Test (MUST) field experiment in urban like environment. Brief details of these experiments and associated numerical (i.e. CFD) simulation setup to compute the adjoint functions are given as follows.

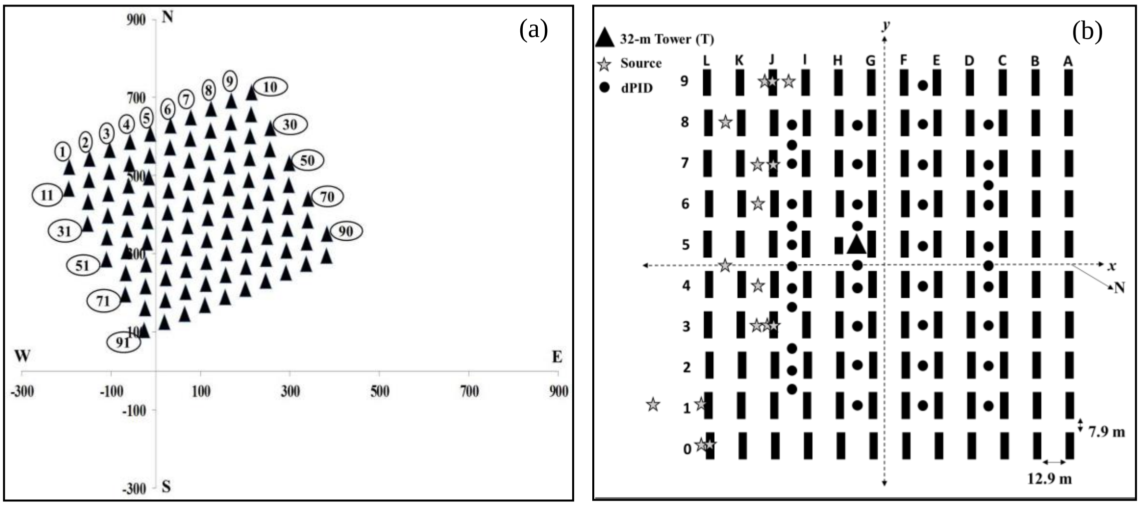

Figure 1. Schematic diagrams of (a) Fusion Field Trial (FFT-07) tracer experiment in flat terrain and (b) Mock Urban Setting Test (MUST) field experiment in urban like enviornment.

Fusion Field Trial 2007 (FFT-07) experiment

Recently, a short range (~500 m), comprehensive tracer field experiment was conducted in September, 2007 at the U.S. Army's Dugway Proving Ground (DPG), Utah (Storwold, 2007). This highly instrumented test is referred to as Fusing Sensor Information from Observing Networks (FUSION) Field Trial 2007 (FFT-07). This experiment involves various instantaneous, continuous, single as well as multiple point releases in various atmospheric stability conditions varying from neutral to stable, and unstable conditions. In this experiment, a tracer propylene (C_3H_6) was release at 2 m height above the ground surface and the concentrations were measured at 100 fast response digital Photo Ionization Detector (digiPID) samplers arranged in a rectangular staggered grid of area 475 m × 450 m in 10 rows and 10 columns. The digiPID samplers were also deployed at 2 m height above the ground surface. Figure 1(a) shows a schematic diagram of the FFT-07 experiment.

One trail #30 (Date: 20-09-2007) is selected in present study for the identification of a continuous point source in a flat terrain. In this trial, 113.6 l min^{-1} C_3H_6 was continuously released in the atmosphere for ~10 min. The study domain for numerical simulations comprises outer and inner domains of width × length 2000 m × 2000 m and 1000 m × 1000 m, respectively. To ensure a smoothly varying wind flow over the boundary of inner domain, outer domain boundary was kept away from the main test site consisting all the sensors and instruments and thus, size of outer computational domain was considered approximately four times of the inner domain. The heights of inner and outer domains were taken as 100 m and 200 m, respectively. The 3-D unstructured mesh in both domains consists 2644149 grid cells.

Mock Urban Setting Test (MUST) field experiment

For evaluation of the source reconstruction methdology in an urban enviornment, we have used the observations taken from the MUST field experiment conducted at the U.S. Army Dugway Proving Ground (DPG) Horizontal Grid test site (40°12.606' N, -113°10.635' W) from 6-27 September 2001 (Biltoft, 2001). The test site was primarily flat with an averaged momentum roughness length of 0.045 ± 0.0005 m (Yee and Biltoft, 2004). The MUST experiment represents an urban geometry by placing 120 shipping containers (12.2 m × 2.42 m × 2.54 m) arranged in a large array of building-like obstacles in 10 rows and 12 columns (Fig. 1(b)). This experiments was conducted mostly in neutral and stable atmospheric conditions. A detailed description of the meteorological and tracer observations are given in Biltoft (2001) and Yee and Biltoft (2004).

In present study, one trial #2682353 (Date: 25-09-2001) is selected for a continous point source retrieval in an urban-like environment. In this selected case, 225 l min^{-1} C_3H_6 was continuously released in the atmosphere for 15 min from a 5.2 m source height and measured at a height of 1.6 m (at 40 receptors) and 1, 2, 4, 6, 8, 10, 12, and 16 m (at 8 receptors in vertical direction on a single point in the domain) above the ground surface. The mean wind speed and direction during this trial were 4.49 ms^{-1} and -47°, respectively, with stable atmospheric conditions (Obukhov length L_{MO} = 120 m) (Yee and Biltoft, 2004). The simulation domain comprises outer (800 m × 800 m) and inner (nested) (250 m × 225 m) domains. Inner domain contains the urban structure consisting the MUST obstacle array (193 m × 171 m) and keeping the outer domain boundary away from obstacles ensures a smoothly varying wind flow over the inner domain boundary. The heights of the inner and outer domains were taken as 100 m and 200 m, respectively. The 3-D unstructured mesh is chosen for both outer and nested domains that consists a total 2849276 grid cells in the embedded mesh. In an ideal run, all the residuals was considered to be equal or less than $O(10^{-4})$ to ensure a converged solution.

RESULTS AND DISCUSSIONS

The source reconstructions for both FFT-07 and MUST field experiments are carried out with synthetic and real concentrations measurements. Knowing the location $\mathbf{x_0}$ and intesity q_0 of a continuous point source, synthetic measurements are simply generated from the computed retroplumes as $\mu_i^{synt} = q_0\, a_i(\mathbf{x}_0)$. Synthetic measurements are free from any model and instrumental errors and ideal to evaluate a source reconstruction methdology. In case of the synthetic measurments, source parameters (i.e. location, height, intensity) are exactly estimated in flat and urban enviornments in both the experiments. This affirms the mathematical consistenty of the inversion methdology coupled with a CFD apprach. The error in retrieved source location is represented by the Euclidian distance of the retrieved location from the true source.

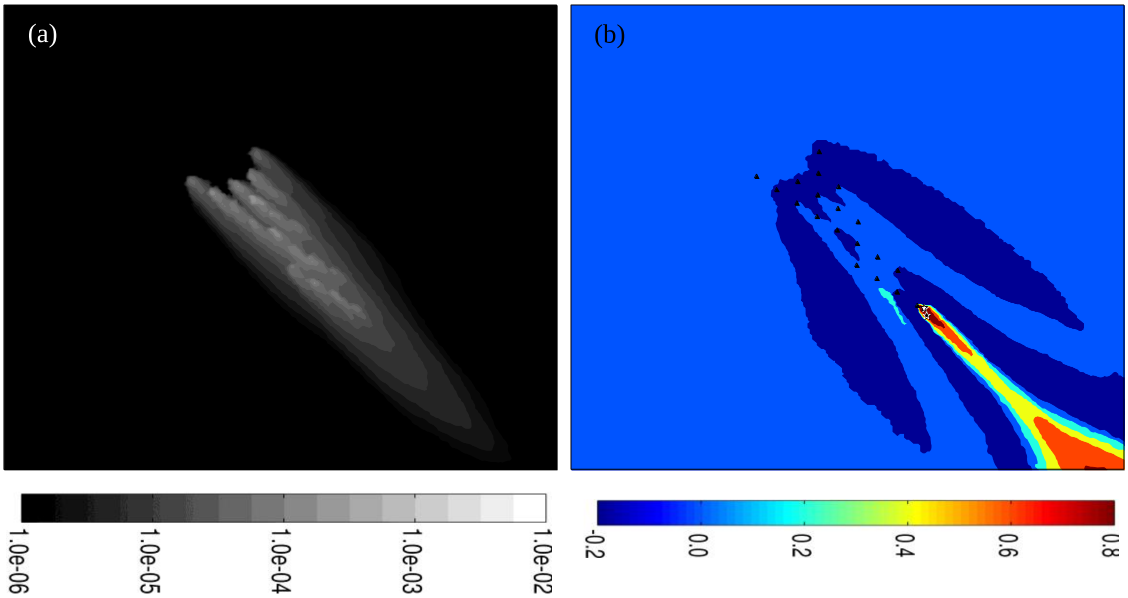

Figure 2. Isopleths of (a) weight function w(**x**) and (b) normalized source estimates $\mathbf{s}^n(\mathbf{x}) = \mathbf{s}(\mathbf{x})/max(\mathbf{s}(\mathbf{x})$ with real concentration measurements in trial 30 of FFT-07 experiment. The black and white filled circles in Figure (b) show the true and estimated source locations, respectively.

Isoplethes of the renormalized weight function in Fig. 2(a) shows the peaked values at the samplers' locations of the non-zero concentrations in trial-30 of FFT-07 experiment. The computed renormalized weight function includes the natural information associated with the sensors and physically interprets the extent of regions seen by the monitoring network. The weight function decreases in upwind direction and shows the lack of visibility for the most distant sources. A distribution of the normalized source estimates is shown in Fig. 2(b) in a horizontal cross-section plane corressponding to the estimated source height. With real concentration measurements, source is retrieved 20.06 m upwind from the true location. The release height is retrieved at 3.125 m above the ground surface, which is close to the true source height 2 m. An overprediction is observed in the retrieved source intensity. The estimated release rate is 284.7 l/min, which is 2.5 times greater than the true source intensity 113.6 l/min in this trial.

Figure 3(a) & (b) show the contour plots of the renormalized weight function and the normalized source

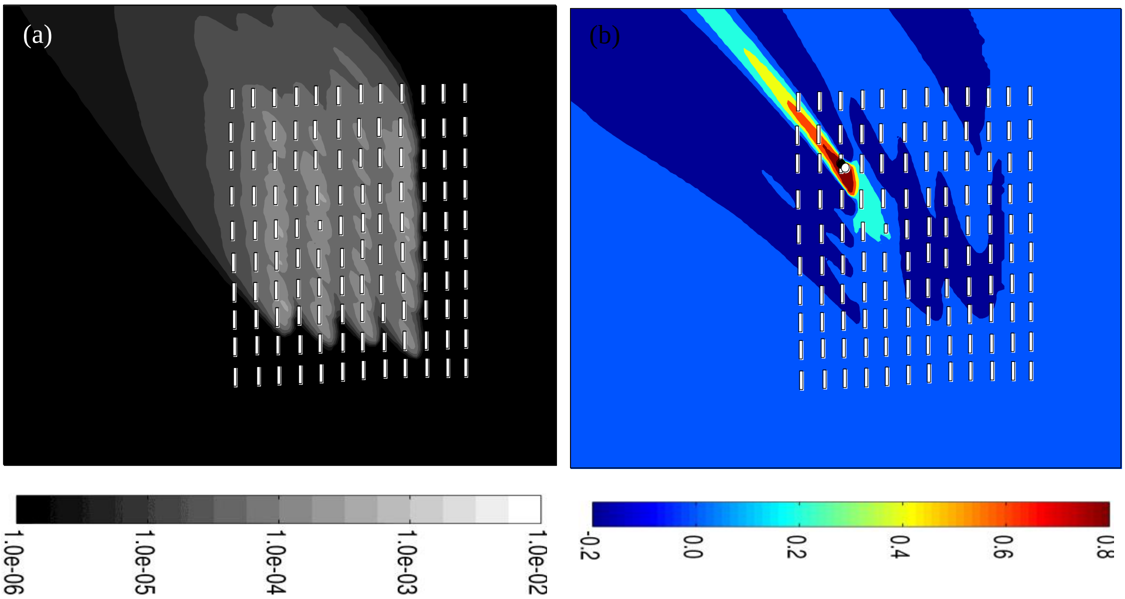

Figure 3. Isopleths of (a) weight function w($\mathbf{x}$) and (b) normalized source estimates $\mathbf{s}^n(\mathbf{x}) = \mathbf{s}(\mathbf{x})/max(\mathbf{s}(\mathbf{x}))$ with real concentration measurements in trial #2682353 of MUST field experiment.

estimates in a horizontal cross-section plane corressponding to the estimated source height in trial #2682353 of MUST experiment. The estimated point source is very close to the true source location (Fig. 3(b)). The Euclidean distance of the estimated source location from the true source is 4.22 m. The release height is estimated at 4.22 m above the ground which is also close to the true source height 5.2 m in this trial. The intensity of the estimated point source is retrieved within a factor of two of the true release rate. The retrieved intensity is 306.12 l/min, which is 1.36 times greater than the true release rate 225 l/min.

CONCLUSIONS

This study describes a methodology to retrieve a continuous point release in 3-dimensional space in urban and non-urban regions and addresses a problem of vertical structure in atmospheric source reconstruction. The methdology is based on the renormalization inversion technique coupled with a CFD approach. The methodology is evaluated with the FFT-07 and MUST field experiments to retrieve the location, height, and strength of a continous point release in flat and urban enviornments, respectively. The source parameters are estimated close to the true source parameters. By estimating the source height along with the other source parameters, this study shows the effectiveness of the renormalization inversion technique coupled with a CFD approach to estimate a continuous point release in urban and non-urban regions.

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