An Urban Scale Inverse Modelling for Retrieving Unknown Elevated Emissions with Building-Resolving Simulations

Pramod Kumar^{a,*}, Sarvesh Kumar Singh^a, Amir-Ali Feiz^a, Pierre Ngae^a

^a*LMEE, Université d'Evry Val-d'Essonne, 40 Rue Du Pelvoux 91020 Courcouronnes, France.*

Abstract

This study illustrates an atmospheric source reconstruction methodology for identification of an unknown continuous point release in the geometrically complex urban environments. The methodology is based on the *renormalization* inversion theory coupled with a building resolving Computational Fluid Dynamics (CFD) 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. An estimation of the release height in a three-dimensional urban environment is relatively more difficult from both technical and computational point of view. Thus, a salient feature of the methodology is to address the problem of vertical structure (i.e. height of a source) in atmospheric source reconstruction in three-dimensional space of an urban region. The inversion methodology presents a way to utilize a CFD model fluidyn-PANACHE in source reconstruction in the urban regions. The described methodology is evaluated with

*Corresponding author.

Email address: `kumar@ufrst.univ-evry.fr` (Pramod Kumar)

20 trials of the Mock Urban Field Setting Test (MUST) field experiment in various atmospheric stability conditions varying from neutral to stable and very stable conditions. The retrieved source parameters in all the 20 trials are estimated close to their true source. The source height is retrieved within a factor of two and four in 55% and 75% of the MUST trials, respectively. The averaged location error for all 20 trials is obtained 14.54 m with a minimum of 3.58 m and maximum of 34.55 m. The averaged estimated release rate for all trials is overpredicted within a factor of 1.48 of the true source intensity and in 85% of the trials, it is retrieved within in factor of two. In source reconstruction with non-zero measurements, it was observed that the use of all concentration measurements instead of only non-zero essentially makes only the small differences in quality of the source reconstruction and gives a little additional information for better constraining the source parameters. A posteriori uncertainty analysis in the retrieved source parameters is also performed by adding a controlled noise in the concentration measurements and the source reconstruction results were also compared with an earlier study based on the stochastic Bayesian approach for identical 14 MUST trials. The study is useful for emergency regulators to detect an unknown accidental or deliberated continuous point releases in urban regions.

Keywords: CFD, Renormalization, Source reconstruction, MUST field experiment, Urban.

1. Introduction

Fast and accurate identification of an unknown atmospheric tracer source in densely populated and geometrically complex urban environments is es-

4 sential to reduce the extent of subsequent exposure and associated mortality
5 caused by an accidental or deliberated incident. An inversion methodology
6 is required to provide information about the locations, height, and emission
7 rates of the unknown sources. A source reconstruction process generally uti-
8 lizes the ambient concentration measurements of a pollutant observed by a
9 finite number of detectors distributed over a region. However, these con-
10 centration measurements, detected over a threshold value of a sensor, alone
11 provide no particular information about the source including its location,
12 height, and release rate.

13 Atmospheric monitoring in conjunction with source reconstruction mod-
14 elling has the potential to detect, locate, and quantify the localised emissions
15 into the atmosphere (Luhar et al., 2014). In recent years, the problem of iden-
16 tifying an unknown source on small, medium or large scales is discussed in
17 several studies in the literature (Penenko et al., 2002; Issartel, 2005; Boc-
18 quet, 2005; Haupt et al., 2006; Keats et al., 2007; Chow et al., 2008; Sharan
19 et al., 2009; Kovalets et al., 2011; Winiarek et al., 2012; Luhar et al., 2014;
20 Yee et al., 2014; Turbelin et al., 2014; Singh et al., 2015a,b; Kumar et al.,
21 2015b, etc.). These source reconstruction methodologies generally required a
22 numerical dispersion or adjoint model, which prerequisite the realistic wind-
23 field in a computational domain. The consideration of a constant flow-field
24 throughout a region is sufficient to compute the adjoint functions in flat and
25 homogeneous terrains, however, it is not as adequate in urban regions. The
26 computation of the realistic flow-fields in urban regions is difficult due to the
27 impacts of local topography, terrain conditions, buildings and other geometri-
28 cal structures. Buildings in urban regions alter the flow-field, causes updrafts

29 and downdrafts, channeling flow between buildings areas of calm winds ad-
 30 jacent to strong winds, etc. (Brown, 2004). However, the building-resolving
 31 Computational Fluid Dynamics (CFD) models, that solve the Navier-Stokes
 32 fluid dynamics equations using a small grid size (of the order 1 m or even
 33 less) over the complex terrains, can resolve the realistic flow-field in urban re-
 34 gions (Hanna et al., 2004; Kumar et al., 2015a). Accordingly, a CFD model’s
 35 simulated realistic flow-field in urban regions can be utilize in the dispersion
 36 or adjoint models in a source reconstruction process.

37 Recently, Kumar et al. (2015b) described a source reconstruction method-
 38 ology for the identification of an unknown continuous point source located at
 39 the ground level or at a horizontal plane corresponding to a known or prede-
 40 fined altitude above the ground surface in an urban area. This methodology
 41 was based on a recently proposed deterministic *renormalization* inversion
 42 technique (Issartel et al., 2007), coupled with a CFD modelling approach in
 43 two-dimensional space in an urban area. However, in this study, the problem
 44 of vertical structure (i.e. height of a source) in atmospheric source recon-
 45 struction in three-dimensional space of an urban area is not addressed. In
 46 reality, an altitude of a release (i.e. source height) is also not known and
 47 required to estimate along with the projected release location on the ground
 48 surface and the release rate. However, the estimation of the release height in
 49 a three-dimensional urban environment is relatively more difficult from both
 50 technical and computational point of view. First, the complexity arises due
 51 to unresolved vertical structure of the flow and plumes in the urban regions
 52 in different atmospheric stability, terrain, and meteorological conditions that
 53 affect the feasibility of the source estimation. Second, when the number of

54 unknown parameters increases, the computational cost and the complexity of
55 the inversion technique increases. However, the estimation of release height
56 is important along with the projected release location on the ground and
57 intensity, especially when a gas leak or accidental release is elevated or from
58 the rooftops in an urban area.

59 Thus, the objective of the study reported here is to formulate an inverse
60 atmospheric modelling to estimate the effective release height, along with
61 the projected release location on the ground, and strength of an unknown
62 continuous point source in an urban environment. This study addressed the
63 problem of vertical structure in atmospheric source reconstruction in an ur-
64 ban area. The source reconstruction methodology is based on the renormal-
65 ization inversion theory combined with a building resolving CFD approach
66 in three-dimensional space in an urban area. In framework of the inver-
67 sion methodology, a CFD model fluidyn-PANACHE is used for this purpose.
68 This is the first application of the renormalization inversion theory to esti-
69 mate the height of an unknown continuous point source in an urban envi-
70 ronment. The methodology is evaluated with 20 trials of the Mock Urban
71 Setting Test (MUST) field experiment in an urban like environment in var-
72 ious atmospheric stability conditions. The MUST field data is suitable here
73 for the evaluation purpose because the source height and its locations were
74 altered from trial to trial and it can illustrate its applicability to real-world
75 source reconstruction problems in the urban environments.

2. Inverse atmospheric modelling for source retrieval

To estimate the source parameters (i.e. release height, location and intensity), an inversion approach generally uses a finite set of the concentration measurements at some receptors and a source-receptor relationship. This study explores the feasibility of using the *renormalization* based inversion approach (Issartel, 2005) for three-dimensional (3-D) reconstruction of a continuous atmospheric point source in an urban environment. The adjoint source-receptor relationship is used here and it required an atmospheric dispersion or adjoint model and flow-field in complex urban regions. An adjoint model should properly accounts for the effects of flow inhomogeneities due to the buildings and other obstacles on dispersion in urban regions. The inversion technique is described here for an elevated continuous emission in 3-D discretized space and thus, the time coordinates are ignored in the formulations. However, the technique presented here could be made 4-dimensional to additionally identify the time of an instantaneous point release in the urban regions.

2.1. Source-receptor relationship

Assuming that a domain is discretized in N number of grid cells in a 3-dimensional space $\mathbf{x} = (x, y, z)$ and $\mathbf{s} \in \mathbb{R}^N$ is an unknown source vector to determine. A finite set of m concentration measurements $\boldsymbol{\mu} = (\mu_1, \mu_2, \dots, \mu_m)^T \in \mathbb{R}^m$ are assumed linear to the emission $\mathbf{s}$. In a receptor-oriented approach for the source reconstruction that includes solution of an adjoint transport equation (Pudykiewicz, 1998; Hourdin and Talagrand, 2006), the 3-D atmospheric coupling coefficient $a_i(\mathbf{x})$ corresponding to each

receptor formed a source-receptor relationship. The correspondence between the unknown emissions $\mathbf{s}$ and the measurements $\boldsymbol{\mu}$ is defined with the adjoint functions $a_i(\mathbf{x})$

$$\boldsymbol{\mu} = \mathbf{A}\mathbf{s} + \boldsymbol{\epsilon} \quad (1)$$

where $\mathbf{A} \in \mathbb{R}^{m \times N}$ is a sensitivity matrix composed of the m time-invariant adjoint functions $a_i(\mathbf{x})$ in a 3-D space and the source vector $\mathbf{s}$ represents discrete components of the unknown emission. The term $\boldsymbol{\epsilon} \in \mathbb{R}^m$ represents the total measurement error and it comprises the error due to (i) the detector limitations and (ii) the limited representativity of a dispersion or adjoint model utilized to describe the correspondence between the emissions and the measurements. The volume elements of each grid-cell is incorporated in $\mathbf{s}$, so that it represents the total activity released in a grid-cell. Each column vector of matrix $\mathbf{A} = [\mathbf{a}(\mathbf{x}_1), \mathbf{a}(\mathbf{x}_2), \dots, \mathbf{a}(\mathbf{x}_N)]$, where $\mathbf{a}(\mathbf{x}_i) \in \mathbb{R}^m$, reflects the potential sensitivity of a grid cell with respect to all m concentration measurements.

For a simple demonstration of the inversion process, a fit to the pollutant concentration $\boldsymbol{\mu}$ at each detector with avail of the sensitivity matrix $\mathbf{A}$ can produce a source vector $\mathbf{s}$. However, the inverse problem to estimate $\mathbf{s}$ in Eq. (1) is an ill-posed and highly underdetermined in nature as $m \ll N$. Indeed, in a very general case where the point detectors have a negligible volume compared to the dimensions of the problem, the adjoint functions are singular (with infinite (very large) value) at the position of detectors and have strong concentration gradients (Issartel, 2005; Saide et al., 2011). These peaks are interpreted as artificial information and are regularized by using

123 the *renormalization* assimilation process (Issartel et al., 2007).

124 2.2. Renormalized assimilation

125 Renormalization inversion theory was originally developed for the estima-
 126 tion of distributed emission sources $\mathbf{s}$ from the concentration measurements
 127 (Issartel et al., 2007) and extended to estimate the point source (Sharan et al.,
 128 2009). A salient feature of the theory is its distinction of two geometries of
 129 the environment where emissions occur. The *renormalization* inversion the-
 130 ory was further extended to estimate a 2-D ground level point release (or
 131 source in a horizontal plane corresponding to a predefined or known vertical
 132 plane) in an urban area (Kumar et al., 2015b).

133 Due to diffusive nature of the transport and strong concentration gra-
 134 dients around the measurement cells, the sensitivity matrix $\mathbf{A}$ is associated
 135 with peaks at the sensitivity vectors coinciding with the cells containing
 136 measurements (Issartel et al., 2007). These peaks generate artifacts at the
 137 point of measurements, that returns unsatisfactory estimates, and need to
 138 be regularized. The regularization of peaks in the *renormalization* source
 139 reconstruction process is purely based on the computation of a weight func-
 140 tion $\mathbf{W} \in \mathbb{R}^{N \times N}$. The weight matrix $\mathbf{W}$ is purely diagonal in nature with
 141 elements $w_{jj} > 0$ such that $\sum_{i=1}^N w_{jj} = m$. The introduction of $\mathbf{W}$ modifies the
 142 sensitivity matrix as $\mathbf{A}_w = \mathbf{A}\mathbf{W}^{-1}$ and thus, the Eq. (1) transforms to :

$$\boldsymbol{\mu} = \mathbf{A}_w \mathbf{W} \mathbf{s} + \boldsymbol{\epsilon}. \quad (2)$$

143 In order to estimate the unknown source vector $\mathbf{s}$, a constrained opti-
 144 mization problem can be formed to minimize a cost function $J(\mathbf{s}) = \mathbf{s}^T \mathbf{W} \mathbf{s}$,

145 subjected to a constraint $\boldsymbol{\epsilon} = \boldsymbol{\mu} - \mathbf{A}_w \mathbf{W} \mathbf{s} = 0$. The optimization problem
 146 can be solved by applying the method of Lagrange multipliers and a unique
 147 least-norm estimate ($\mathbf{s}_w$) of $\mathbf{s}$ can be derived as (Appendix A) :

$$\mathbf{s}_w = \mathbf{A}_w^T \mathbf{H}_w^{-1} \boldsymbol{\mu} \quad (3)$$

148 where $\mathbf{H}_w^{-1}$ is the inverse of a symmetric positive definite *Gram matrix* $\mathbf{H}_w =$
 149 $\mathbf{A}_w \mathbf{W} \mathbf{A}_w^T$.

150 The least-norm estimate $\mathbf{s}_w$ in Eq. (3) required to determine the appro-
 151 priate elements w_{ij} of the weight matrix $\mathbf{W}$. Issartel (2005) showed that a
 152 unique weight matrix $\mathbf{W}$ exists and satisfies the following conditions :

- (i) $w_{jj} > 0$, (ii) $trace(\mathbf{W}) = m$, and
 - (iii) the diagonal terms of $\mathbf{A}_w^T \mathbf{H}_w^{-1} \mathbf{A}_w$ are unity,
- i.e. $\mathbf{a}_w^T(\mathbf{x}) \mathbf{H}_w^{-1} \mathbf{a}_w(\mathbf{x}) \equiv 1$, or equivalently $trace(\mathbf{A}_w^T \mathbf{H}_w^{-1} \mathbf{A}_w) = N$.
- (4)

153 $\mathbf{W}$ satisfies an appropriate optimality condition (iii) and this criterion is
 154 also called as renormalizing condition (Issartel et al., 2007). An iterative
 155 algorithm to compute the weight coefficient $w(\mathbf{x})$ at location $\mathbf{x}$ is described
 156 as (Issartel et al., 2007) :

$$w_0(\mathbf{x}) = 1, \quad \text{and} \quad w_{k+1}(\mathbf{x}) = w_k(\mathbf{x}) \sqrt{\mathbf{a}_{wk}^T(\mathbf{x}) \mathbf{H}_{wk}^{-1} \mathbf{a}_{wk}(\mathbf{x})} \quad (5)$$

157 where k is an iteration step. The weights $w(\mathbf{x})$, best removing inversion
 158 artifacts, called the renormalizing weights. The renormalized weight function
 159 $w(\mathbf{x})$ also referred to as a visibility function, as it is useful in the physical

160 interpretation of the extent of the regions seen by the monitoring network
 161 (Sharan et al., 2009). The visibility function indicates how well a possible
 162 location of a release is observed and, thus, it provides a simple criterion for
 163 optimizing the design of the monitoring network.

164 2.2.1. Point source retrieval

165 A continuous point source is generally characterized by an intensity q_0
 166 in unit amount of tracer per unit time and a location $\mathbf{x}_0 = (x_0, y_0, z_0)$ in a
 167 3-D space, where z_0 is the release height and (x_0, y_0) is the projected release
 168 location on the ground surface. Thus, assuming a priori information about
 169 the nature of release, i.e. from a point source, it reduces the number of
 170 unknowns to four parameters (q_0 , x_0 , y_0 , and z_0) to estimate. A continuous
 171 point source can be defined by $s(\mathbf{x}) = q_0\delta(\mathbf{x} - \mathbf{x}_0)$, where δ is the Dirac delta
 172 function. Substituting this formula of a point source in Eq. (2) gives (Sharan
 173 et al., 2009) :

$$\boldsymbol{\mu} = q_0\mathbf{a}_w(\mathbf{x}_0)w(\mathbf{x}_0) + \boldsymbol{\epsilon}. \quad (6)$$

174 where $\mathbf{a}_w(\mathbf{x}_0) = \mathbf{a}(\mathbf{x}_0)/w(\mathbf{x}_0)$. Thus, $\mathbf{s}_w$ from Eq. (3) can be described as :

$$\mathbf{s}_w = q_0w(\mathbf{x}_0)\mathbf{A}_w^T\mathbf{H}_w^{-1}\mathbf{a}_w(\mathbf{x}_0). \quad (7)$$

175 Renormalization condition (*iii*) from Eq. (4) shows that $\mathbf{s}_w$ in Eq. (7) attains
 176 its maximum only at a location $\mathbf{x} = \mathbf{x}_0$ (because $\mathbf{a}_w^T(\mathbf{x})\mathbf{H}_w^{-1}\mathbf{a}_w(\mathbf{x}_0) = 1$ only
 177 when $\mathbf{x} = \mathbf{x}_0$). Thus, the source location ($\mathbf{x}_0$) can be estimated on a map
 178 by searching the *maximum* of $\mathbf{s}_w$. Once the source location $\mathbf{x}_0$ is estimated,
 179 its intensity at $\mathbf{x} = \mathbf{x}_0$ is determined from Eq. (7) as :

$$q_0 = s_w(\mathbf{x}_0)/w(\mathbf{x}_0). \quad (8)$$

180 2.3. Adjoint functions in urban environments

181 Flow-field in urban environments is not homogeneous like generally con-
 182 sidered for the flat terrains and it often diverted into unexpected directions
 183 by the building and other structures. The unsteady and inhomogeneous
 184 flow effect, triggered by the presence of buildings and other geometries, is
 185 an influencing factor on the dispersion in urban or industrial regions. Con-
 186 sideration of the constant wind-field throughout a domain to compute the
 187 adjoint functions from Gaussian or analytical dispersion models is not ap-
 188 propriate in urban regions (Winiarek, 2014; Kumar et al., 2015a). Compared
 189 with simple Gaussian dispersion models or other analytical or empirical ap-
 190 proximations, CFD models efficiently predict the obstacles influence on wind
 191 patterns and pollutant cloud shapes in complex urban environments (Kumar
 192 et al., 2015a). Thus, a CFD model fluidyn-PANACHE is first used to simu-
 193 late the flow-field in an urban area. This flow-field is then used to compute
 194 the adjoint functions.

195 2.3.1. Description of the CFD model: fluidyn-PANACHE

196 A description of the CFD model fluidyn-PANACHE is given in Fluidyn-
 197 PANACHE (2010) and Kumar et al. (2015a). The fluidyn-PANACHE solves
 198 the Reynolds Averaged Navier-Stokes (N-S) (RANS) fluid dynamics equa-
 199 tions, along with the equations describing conservation of species concentra-
 200 tion, mass, heat transfer and energy for a mixture of ideal gases using finite
 201 volume numerical techniques. It includes an unsteady RANS CFD solution

202 that refers to ensemble-averaging of the N-S equations and resolves only the
 203 unsteady mean-flow structures, while it models the turbulence. A built-in
 204 automatic 3-D mesh generator is included in the fluidyn-PANACHE that can
 205 create the finite-volume mesh around obstacles and body-fitting the terrain
 206 undulations.

207 In fluidyn-PANACHE, ideal gas law is used for the thermodynamic model
 208 of mixture of gases. Air is modelled as the moist air with effective properties
 209 of the mixture of dry air and water vapour. The Reynolds stresses are mod-
 210 elled using a linear eddy viscosity model (LEVM) (Ferziger and Peric, 2002).
 211 Atmospheric turbulence due to shear (flow over ground or over obstacles) as
 212 well as due to thermal effects (solar heating of ground, buoyant plumes) is
 213 modelled with a two-equations prognostic $k-\epsilon$ model that solves an equation
 214 for the turbulent kinetic energy (k) and another equation for its dissipation
 215 rate (ϵ). The atmospheric boundary layer (ABL) processes are built-in the
 216 CFD code with different numerical models. The CFD model accounts the sta-
 217 bility effects through inflow boundary conditions and includes an ABL model
 218 that serves as the interface between the meteorological observations and the
 219 boundary conditions. The ABL model is composed of two parts: (i) a mi-
 220 crometeorology model that computes fundamental physical characteristics of
 221 the ABL from routine meteorological observations and (ii) a boundary layer
 222 model for describing the vertical profiles of wind speed, temperature, and
 223 turbulence. Dispersion of gases is modelled by solving the full conservation
 224 equations governing the transport of species concentration. The buoyancy
 225 model is used to parametrize the body force term in the N-S equations. To
 226 couple the pressure and momentum equations in the numerical computa-

227 tions, the Semi-Implicit Method for Pressure Linked Equations-Consistent
228 (SIMPLEC or SIMPLE-Consistent) algorithm (Van Doormaal and Raithby,
229 1984) is utilized.

230 2.3.2. $k - \epsilon$ turbulence model

231 To resolve the turbulent structure in a computational domain, a modified
232 standard $k - \epsilon$ turbulence model is used. The $k - \epsilon$ model is a two-equation
233 linear eddy viscosity model and describes the mean of a turbulent flow. It
234 solves the transport equations for turbulent kinetic energy, k and its dis-
235 sipation rate, ϵ . The fluidyn-PANACHE implementation of this model is
236 derived from the standard high-Reynolds number (Re) form with corrections
237 for buoyancy and compressibility (Launder, 2004; Hanjalic, 2005). The $k - \epsilon$
238 model computes the length and time scales from the local turbulence charac-
239 teristics. Thus, it can model the turbulent flows subjected to both mechanical
240 shear (obstacles, terrain undulations, canopy) as well as buoyancy (stability
241 and buoyant/heavy gas plumes).

242 2.3.3. Boundary conditions

243 Recently, Kumar et al. (2015a) discussed the use of proper inflow bound-
244 ary conditions in a CFD model for dispersion of pollutant in an urban area.
245 The lateral boundaries of the domain are treated as inflow and outflow bound-
246 aries based on the direction of the wind with respect to the domain boundary.
247 The top boundary is treated as an outflow boundary and a no-slip bottom
248 boundary condition is defined at the ground surface where the velocity com-
249 ponents are set to zero. Standard wall functions (Hanjalic, 2005) are used
250 to compute the drag forces on solid walls in a turbulent boundary layer.

251 At the inflow boundary, velocity, temperature, and turbulence variables are
 252 specified as follows :

253 (i) *Wind profile* : Gryning et al. (2007) wind profile in stable and neutral
 254 conditions is used. These profiles are composed of the three different
 255 length scales in surface, middle, and upper layers of the ABL, and is
 256 applicable in the entire ABL. As the Gryning et al. (2007) wind profile
 257 is not suitable for very stable atmospheric conditions, a wind profile
 258 based on a similarity function proposed by Beljaars and Holtslag (1991)
 259 is used in extreme stability conditions due to its applicability in these
 260 stability conditions (Sharan and Kumar, 2010).

261 (ii) *Temperature profile* : Monin-Obukhov similarity theory based logarithmic
 262 temperature profile is used to describe its vertical variation in neu-
 263 tral and stable conditions.

264 (iii) *Turbulence profiles* : The profiles of k and ϵ based on an approximate
 265 analytical solution of one-dimensional $k - \epsilon$ prognostic equation (Yang
 266 et al., 2009) are used for inflow boundary conditions. Coefficients in
 267 these profiles of k and ϵ are estimated based on the observations of k .

268 2.3.4. *Adjoint functions*

269 Adjoint functions are computed in two steps : (i) 3-D converged flow field
 270 ($\mathbf{u}$) was computed from the CFD model, and (ii) by reversing the direction of
 271 wind by 180° , this wind-field is used to solve the adjoint transport equation
 272 (Marchuk, 1995; Pudykiewicz, 1998; Hourdin and Talagrand, 2006):

$$-\frac{\partial r_i}{\partial t} - \mathbf{u} \cdot \nabla r_i - \frac{1}{\rho} \nabla \cdot (\rho \mathbf{K} \nabla r_i) = \sigma_i \quad (9)$$

where r_i is an adjoint function corresponding to the i^{th} measurement μ_i , σ_i is a sampling function associated with μ_i and behave like a source at the receptor locations. The adjoint functions r_i are often called as the retroplumes or sensitivity functions (Issartel, 2005). For concentration observations measured by the detector at a point, the geometry of the source at receptor location is generally considered as a 3-D point source with unit strength in computations of the retroplumes from Eq. (9).

For a continuous release in the atmosphere, adjoint functions become steady with respect to the time. Thus, the time dimension can be discarded and the retroplumes are the function of space variables $\mathbf{x}$ only, i.e. $r_i(x, y, z, t) = a_i(x, y, z)$.

3. Mock Urban Setting Test (MUST) field experiment

The Mock Urban Setting Test (MUST) field experimental was conducted from 6th to 27th September, 2001 at the U.S. Army Dugway Proving Ground (DPG) Horizontal Grid test site (40°12.606'N, -113°10.635'W) (Biltoft, 2001). In this experiment, an urban like environment was created by placing 120 shipping containers (each 12.2 m long $\times$ 2.42 m wide $\times$ 2.54 m high) in 10 rows and 12 columns. These containers formed an approximately 200 m $\times$ 200 m region of urban like geometry. Figure 1 shows a layout of the arrangement of the obstacles array in this field experiment. The atmospheric conditions varied from neutral to stable and very stable during the releases in this experiment.

In this study, 20 trials of the MUST experiment are selected for the source reconstruction in various atmospheric conditions. Table 1 presents

297 the meteorological, turbulence, and source parameters in each selected trial.
 298 The values of the meteorological and turbulence parameters are taken from
 299 Yee and Biltoft (2004). In each trial of the MUST experiment, a tracer gas
 300 (C_3H_6) was continuously released for ≈ 15 min from a point source. The
 301 release locations and height were altered slightly from trial to trial, but were
 302 always near the first three rows of obstacles (Fig. 1). The tracer gas was
 303 released at one of the five vertical heights 0.15, 1.3, 1.8, 2.6, and 5.2 m above
 304 the ground surface. The concentrations were measured by 40 Digital photo-
 305 ionization detectors (dPIDs) at 1.6 m above the ground surface, and 8 dPIDs
 306 deployed on eight vertical heights at a single location. The 40 detectors at
 307 1.6 m were arranged in four horizontal sampling lines approximately 25, 60,
 308 95, and 195 m downwind from the release locations (Yee and Biltoft, 2004).
 309 In each trial, 200 s quasi-steady periods were extracted within each 15 min
 310 plume dispersion experiment and the concentration measurements during
 311 these periods are used in the estimation of source parameters.

312 **4. Numerical computations and model application strategy**

313 The horizontal domain for the calculations considered two computational
 314 domains : (i) inner (or nested) domain and (ii) outer domain. The inner
 315 domain is defined a size of 250 m $\times$ 225 m (width $\times$ length) that contains
 316 the MUST urban geometry of a size 193 m $\times$ 171 m. The outer domain is
 317 defined approximately four times (800 m $\times$ 800 m) of the size of inner domain.
 318 The vertical domains extended from ground level up to 100 m and 200 m
 319 for inner and outer domain, respectively. These inner and outer domains
 320 discretized into 56 and 61 vertical levels, respectively. In both domains,

321 lowest 40 vertical levels are set with an uniform 0.25 m grid spacing that
 322 formed the lowest 10 m of the vertical domains. Above the 10 m level, the
 323 vertical grid spacing are set to uniform 2 m (5 vertical levels between 10 m
 324 - 20 m), 5 m (4 levels between 20 m - 40 m), 10 m (6 levels between 40 m -
 325 100 m), and, 20 m (5 levels between 100 m - 200 m for outer domain only).
 326 3-D unstructured mesh is generated in both the domains. A grid sensitivity
 327 analysis with different mesh resolutions is performed to adapt the mesh for
 328 numerical simulation. With refined mesh in the inner domain, near to the
 329 obstacles and at locations of the receptors, the 3-D computational domain
 330 consists of a total 2849276 grid cells.

331 The coefficients in approximate analytical profiles of k and ϵ for inflow
 332 boundary conditions are estimated based on the observations of k measured
 333 from three horizontal two-dimensional (2-D) sonic anemometer at a 16 m
 334 telescoping pneumatic mast (located 30.5 m upwind of the front obstacle
 335 array). The calculations of the adjoint functions are performed in two steps
 336 of the fluidyn-PANACHE. In first step, steady wind-field is computed for
 337 each trial of the MUST experiment. In second step, this computed wind-
 338 field is reversed by 180° and used in the atmospheric dispersion equation to
 339 compute the adjoint function corresponding to each measurement.

340 The source parameters (q_0, x_0, y_0, z_0) from the *renormalization* inversion
 341 theory coupled with the building resolving CFD modelling approach in each
 342 MUST trial are estimated in following steps:

343 *Step 1* : Computation of the flow-field $\mathbf{u}(\mathbf{x})$ in 3-D urban domain using the
 344 CFD model fluidyn-PANACHE,

345 *Step 2* : Computation of the adjoint functions $a_i(\mathbf{x})$ corresponding to each

346 measurement using 180° reversed flow-field $-\mathbf{u}(\mathbf{x})$ in a dispersion
 347 model,

348 *Step 3* : Computation of a matrix $\mathbf{A} \in \mathbb{R}^{m \times N}$ from m adjoint functions $a_i(\mathbf{x})$,
 349 and *Gram matrix* $\mathbf{H} = \mathbf{A}\mathbf{A}^T$,

350 *Step 4* : Computation of the weight matrix $\mathbf{W} \in \mathbb{R}^{N \times N}$ with an iterative pro-
 351 cess that generates the matrices $\mathbf{A}_w = \mathbf{A}\mathbf{W}^{-1}$ and $\mathbf{H}_w = \mathbf{A}_w\mathbf{W}\mathbf{A}_w^T$,

352 *Step 5* : Computation of the source vector $\mathbf{s}_w = \mathbf{A}_w^T\mathbf{H}_w^{-1}\boldsymbol{\mu}$,

353 *Step 6* : Search for a location $\mathbf{x}_0 = (x_0, y_0, z_0)$ corresponds to the maximum
 354 of $\mathbf{s}_w$ in 3-D domain, and

355 *Step 7* : Calculate the source intensity $q_0 = s_w(\mathbf{x}_0)/w(\mathbf{x}_0)$ at $\mathbf{x} = \mathbf{x}_0$.

356 The weight matrix $\mathbf{W}$ is attained with an accuracy of $O(10^{-6})$ within 24
 357 iterations from the iterative algorithm described in section 2.2. The compu-
 358 tational methodology for the source reconstruction was programmed in For-
 359 tran. After computing the wind-field and adjoint functions from the CFD
 360 model, the computational time for retrieval of source parameters in 3-D space
 361 for each MUST trial was ≈ 10 min on a single core of a CentOS release 6.5
 362 machine consisting of Intel(R) Xeon(R) CPU E5-2695 v2 @ 2.40GHz.

363 Prior to discussion of the source reconstruction results, main assumptions
 364 in the inversion methodology formulation are listed as : (i) the number of
 365 sources is known a priori, i.e. single source, (ii) the source emissions are
 366 steady, i.e. time invariant emission rate, and (iii) nature of the source, i.e.
 367 point release. The steady state conditions have been assumed in the present
 368 case, which is appropriate given the scale of the MUST field experiment.

369 However, this is not likely to be true in real-world urban areas, which are
 370 usually of much bigger scale, so the time dependence (of meteorology and
 371 dispersion) within the domain would be important in such cases, especially
 372 when the averaging times are smaller than the scale of the domain.

373 5. Results and discussions

374 Source parameters are estimated using (i) synthetic and (ii) real concen-
 375 tration measurements in each trial of the MUST experiment. The synthetic
 376 measurements are the modelled concentrations which are used as a first check
 377 to test if the inverse model can reproduce the emission used in the deriva-
 378 tion of these concentrations. In both types of measurements, source recon-
 379 struction are performed for (i) all measurements generated by 40 detectors
 380 (including zero and non-zero concentrations) and (ii) only non-zero measure-
 381 ments. Synthetic measurements are free from any instrumental, background,
 382 and model errors, and are ideal to validate an inversion methodology for
 383 source reconstruction. Knowing the source location ($\mathbf{x}_s$) and its intensity
 384 q_s in a 3-D domain, synthetic measurements are essentially computed by
 385 $\mu_i = q_s a_i(\mathbf{x}_s)$, where $a_i(\mathbf{x}_s)$ is a value of the adjoint function corresponding
 386 to the i^{th} receptor at known source location $\mathbf{x}_s$. In each trial of the MUST
 387 experiment, source parameters (*i.e.* x_0, y_0, z_0, q_0) are exactly estimated with
 388 all and non-zero synthetic concentration measurements and this affirms the
 389 mathematical consistency of the described source reconstruction methodol-
 390 ogy in 3-D space of an urban environment.

391 For real concentration measurements, Figure 2 shows the isopleths of
 392 the visibility function $w(\mathbf{x})$ (m^{-2}) and normalized source estimate, $s_w^n(\mathbf{x}) =$

393 $s_w(\mathbf{x})/\max(\mathbf{s}_w)$ in the horizontal planes corresponding to the estimated effec-
 394 tive source heights (z_0) for five representative trials 3, 9, 11, 15, and 16. These
 395 trials are corresponding to one trial each from all five true release heights (i.e.
 396 source height (z_s) = 0.15 m, 1.3 m, 1.8 m, 2.6 m, and 5.2 m, in trials 3, 16,
 397 11, 9, and 15, respectively) in the MUST field experiment. Also, these trials
 398 represent all atmospheric stability conditions (i.e. neutral, stable, and very
 399 stable) observed during the experiment. The isopleths of the weight function
 400 and the normalized source estimate for all 20 trials are shown in Supporting
 401 Information (SI) Figures S1.1, S1.2, S1.3, & S1.4. In these Figures (Figures
 402 2, & S1), the contour plots of the source reconstruction results are shown for
 403 (i) all measurements, and (ii) only non-zero measurements.

404 Table 2 presents the source reconstruction results in terms of (i) the error
 405 in retrieved source location (location error) (E_L), (ii) the estimated effec-
 406 tive release height (z_0), and (iii) the estimated source intensity (q_0). The
 407 retrieved source location error (E_L) represents the Euclidean distance of the
 408 estimated source location from its true release location. The ratios (q_0/q_s)
 409 of the estimated (q_0) and the true source release rate (q_s) are also presented
 410 for each trial in Table 2. The results in Table 2 are presented for (i) all mea-
 411 surements and (ii) only non-zero measurements. Variation of the number of
 412 non-zero concentration measurements and meteorological and atmospheric
 413 stability conditions in each MUST trial make the retrieval features different.

414 The isopleths of the renormalized weight function in Figures 2(a) & S1(a)
 415 show the extent of visibility seen by the monitoring network in the horizon-
 416 tal planes corresponding to the estimated effective source heights. It distin-
 417 guishes the well and poorly seen regions for the source retrieval. The prob-

418 ability of a source to be identified is maximum in a well seen region of larger
 419 magnitudes of the visibility function and vice versa. It is worth mentioning
 420 here that the computations of the visibility function are independent of the
 421 concentration measurements. Its computation utilizes only the adjoint func-
 422 tions corresponding to the detectors deployed in a monitoring arrangement
 423 and thus, apparently depends on the geometry of a monitoring network. The
 424 visibility function attains maximum value at location of the detectors. The
 425 distribution of visibility function in the MUST computational domain in Fig-
 426 ures 2(a) & S1(a) exhibits that its magnitude decreases in upwind direction
 427 of the monitoring network and vanishes at the most distant regions. Neg-
 428 ligible magnitudes of the visibility function in downwind of the monitoring
 429 network diminishes the possibility of a sought source in this region.

430 The use of all concentration measurements instead of only non-zero es-
 431 sentially makes the negligible differences in the quality of the source recon-
 432 struction (Table 2, Figures 2 & S1). It suggests that the zero concentrations
 433 measurements gave a little additional information for better constraining the
 434 source parameters. Irrespective of the varying atmospheric stability condi-
 435 tions in all the trials, the source reconstruction results in 3-D space are well
 436 obtained in urban environment of the MUST field experiment.

437 With real concentration measurements, the contour plots in Figures 2(b)
 438 & S1(b) show the distribution of the normalized source estimate in a hor-
 439 izontal plane corresponding to an altitude of the estimated effective source
 440 height (z_0) above the ground surface. The location error in Table 2 and the
 441 isopleths of $s_w^n(\mathbf{x})$ in Figures 2(b) & S1(b) exhibit that the retrieved source
 442 location in each MUST trial is close to the true release location. With all

concentration measurements, the location error is attained with an average of 14.54 m, with minimum in trial 16 ($E_L = 3.58$ m) and maximum in trial 20 ($E_L = 34.55$ m) (Table 2). The minimum location error is attained in trial 15 ($E_L = 2.96$ m) with an averaged location error of 14.50 m using only the non-zero concentration measurements (Table 2).

The source intensity (q_0) is retrieved within a factor of two in $\approx 85\%$ and $\approx 80\%$ trials of the MUST experiment with all and non-zero measurements, respectively. For all trials, the averaged estimated release rate with all measurements is overpredicted within a factor of 1.48 of the true source intensity, and a comparable overestimation (*i.e.* the averaged $q_0/q_s = 1.49$) is also obtained with only non-zero measurements. In trial 2, the retrieved source intensity is largely overestimated within an factor of 4.5 of the true release rate (Table 2). A slight overestimation of the intensity from a factor of two (*i.e.* $q_0/q_s = 2.43$) is obtained in trial 6. Also, in trial 7, q_0 is slightly underestimated from a factor of two of the true release rate (q_s) with all (*i.e.* $q_0/q_s = 0.41$) and non-zero measurements (*i.e.* $q_0/q_s = 0.45$) (Table 2).

The tracer gas in all these trials of the MUST field experiment was released at one of the five vertical heights 0.15 m, 1.3 m, 1.8 m, 2.6 m, and 5.2 m above the ground surface. In 55% and 75% of the trials, the source height is estimated respectively within a factor of two and four in 3-D space of MUST urban environment (Table 2). To take the full advantage of different release heights with different projected locations on the ground surface in this field experiment, 3-D source reconstructions results in the trials with each particular release height are discussed separately in the following subsections.

467 *5.1. Trials with ground level release at $z_s = 0.15$ m*

468 In seven trials 1, 2, 3, 6, 7, 12, & 13, the tracer C_3H_6 was emitted at 0.15
469 m above the ground surface (Table 2) and thus, these trials can be considered
470 corresponding to the ground level releases. These trials were also associated
471 with various atmospheric stability conditions observed during the experiment
472 (neutral: 12, stable: 1, 2, 6, 7, & 13, very stable: 3) (Table 1). With all con-
473 centration measurements, the source height is well retrieved (at $z_0 = 0.125$
474 m) in two trials 7 and 12 in the cells of a horizontal plane corresponds to
475 the lowermost vertical level centred at 0.125 m of the 3-dimensional compu-
476 tational domain. The projected source locations correspond to the estimated
477 release height in these trials 7 & 12 are also retrieved close to their true po-
478 sitions with the location errors (E_L) 12.44 m & 5.43 m, respectively. The
479 source intensity in trial 12 is within a factor of two ($q_0/q_s = 0.86$); whereas,
480 it is slightly underestimated from a factor of two in trial 7 ($q_0/q_s = 0.41$)
481 (Table 2). With all and non-zero concentration measurements, the averaged
482 locations error in all 7 trials corresponding to the ground level release is 14.02
483 m and 13.91 m, respectively. The release rate is estimated within a factor of
484 two in $\approx 57\%$ of these trials with all and non-zero measurements.

485 Although, the location and the intensity in trials 1, 3, 7, & 13 are close
486 to the their respective true release parameters, the retrieved source heights
487 were largely overestimated (Table 2). The release heights in 1, 3, 7, & 13 are
488 estimated as 2.38 m, 2.63 m, 2.13 m, & 1.38 m, respectively. In trial 2, the
489 estimated location error, q_0/q_s , and height are 30.57 m, 4.50, and 3.38 m,
490 respectively and it gives a large overestimation of the release rate. Irrespec-
491 tive of the inversion methodology, estimating a source height also depends on

492 accurately resolving the vertical structure of the computed adjoint functions
493 in 3-D space of an urban geometry. Note that the computation of adjoint
494 functions depends on resolving the vertical structure of the urban boundary
495 layer by a CFD model in different atmospheric stability conditions. The ex-
496 treme stable conditions in trial 3 may not be resolving properly the vertical
497 structure of the atmospheric boundary layer and thus, influences the estima-
498 tion of the source height. It is noted that the estimated source parameters
499 in these trials are approximately similar with all and non-zero concentration
500 measurements (Table 2).

501 5.2. Trials with source height $z_s = 1.3$ m

502 The release height in four trials 16, 17, 19, & 20 was 1.3 m, which is
503 approximately half of the height (2.54 m) of the MUST urban geometry. In
504 all these trials, source was located outside upwind face of the MUST urban
505 array. In trials 16 and 20, source was positioned 24 m upwind outside of the
506 MUST array. Whereas, source was located 1 m upwind of a conex container
507 face in trials 17 and 19. In these trials, it is interesting to test the capability of
508 the source reconstruction methodology to identify a source located outside of
509 the urban environment from the concentration measurements observed from
510 the sensors positioned within an urban region.

511 With all measurements, the source intensity in these four trials is esti-
512 mated within a factor of two. The estimated location is also close to the
513 true source position with minimum location error in trial 16 ($E_L = 3.63$ m),
514 maximum in trial 20 ($E_L = 34.55$ m). The averaged location error for these
515 4 trials is 23.12 m and 23.31 m with all and non-zero concentration measure-
516 ments, respectively. The source heights in trials 19 and 20 are estimated as

1.13 m and 1.38 m, respectively, which are close to the true release height (1.3 m). In trials 16 and 17, the release height is estimated as 3.63 m and 4.38 m, respectively, which are within the factors of 2.8 and 3.4, respectively. With non-zero measurements, the estimated source parameters are approximately similar to that retrieved with all measurements; however, the release height in trial 16 is estimated slightly higher ($z_0 = 3.88$ m) and lower in trial 20 ($z_0 = 0.13$ m). Source reconstruction results in these trials exhibit the ability of inversion methodology to retrieve an atmospheric source positioning outside an urban area from the monitoring network within an urban region.

5.3. Trials with source height $z_s = 1.8$ m

In five trials 4, 5, 8, 10, & 11, the release height was 1.8 m, which is approximately two-thirds of the MUST urban height. In this case, atmospheric stability conditions were observed very stable in trials 4 and 5, stable in 8 and 10, and neutral in trial 11 (Table 1). With all concentration measurements, the source heights in three trials 4, 10, & 11 are respectively estimated as 2.88 m, 1.13 m, and 2.13 m, which are within a factor of two of the true release height 1.8 m (Table 2). However, in two trials 5 and 8, the estimated effective release heights (i.e. $z_0 = 0.38$ m) are within a factor of five. In all these trials, the point sources are estimated close to their true positions with an averaged location error of 14.3 m (with all measurements) and 14.56 m (with non-zero measurements) and the intensity is also retrieved within a factor of two (Table 2). It is worth mentioning here also that the estimated source parameters with non-zero concentration measurements are approximately similar to those retrieved with all measurements, except in trial 8 where the retrieved height ($z_0 = 0.13$ m) is lower than $z_0 = 0.38$ m.

542 *5.4. Trials with source height $z_s = 2.6$ m*

543 Rooftop releases at 2.6 m height above the ground surface were conducted
544 in three trials 9, 14 and 18, where source was positioned at roof of the MUST
545 conex. With all and non-zero measurements, the release height in trial 9 is
546 estimated as 3.63 m and in trials 14 and 18, the estimated effective source
547 height is 4.13 m, which are within a factor of two of the true source height 2.6
548 m. Other source parameters in these trials are also estimated close to their
549 true source (Table 2). With all measurements, location errors in trials 9, 14
550 and 18 are 5.3 m, 6.9 m and 12.33 m, respectively. The retrieved intensities
551 are slightly overestimated and are approximately within a factor of 1.57 of the
552 true release rate. With non-zero concentration measurements, the averaged
553 location error is 7.84 m which is slightly smaller than 8.18 m estimated with
554 all measurements. However, the estimated release rates are comparable with
555 all and non-zero measurements in these trials. Source reconstruction results
556 in these trials show the ability of the described inversion methodology to
557 accurately retrieve the rooftop releases in an urban environment.

558 *5.5. Trial with release at $z_s = 5.2$ m*

559 In one trial 15 (trial #2682353), the tracer was released at 5.2 m height
560 above the ground surface, which makes the source height to be approximately
561 twice of the height (2.54 m) of the MUST urban geometry. This trial can be
562 considered as an elevated release case for the source reconstruction in sta-
563 ble atmospheric conditions (the Obukhov length $L = 120$ m). The contour
564 plots of the normalized source estimates in a horizontal cross-section plane
565 corresponding to the estimated source height in Figure 2(b) show that the
566 estimated point source in this trial is very close to the true source location

567 with all and non-zero concentration measurements (Table 2). With all mea-
568 surements, the Euclidean distance of the estimated source location from the
569 true source is 4.22 m. The release height is estimated at 4.38 m above the
570 ground surface which is also close to the true source height 5.2 m in this
571 trial. The intensity of the estimated point source is retrieved within a factor
572 of two of the true release rate. The retrieved intensity is 306.12 l/min, which
573 is 1.36 times greater than the true release rate 225 l/min (Table 2).

574 With non-zero concentration measurements, the source height is esti-
575 mated same as with all measurements. However, a slightly improvement of
576 the location error ($E_L = 2.96$ m) and intensity ($q_0 = 285.57$ l/min, $q_0/q_s =$
577 1.27) is observed (Table 2). The source reconstruction results in this trial
578 show that the described methodology is efficient enough to retrieve the source
579 parameters of an elevated release, even a release high enough than the urban
580 height or from roof of a building, in 3-D space of an urban environment.

581 5.6. *Quantification of posterior uncertainty in estimated source parameters*

582 Characterization and analysis of the uncertainties in estimated source pa-
583 rameters (i.e. location, height, and intensity) is an important part of a source
584 reconstruction process. In reality, insufficiency and noise in the concentra-
585 tion measurements give rise the uncertainty in estimated source parameters.
586 Other main factors that causes the uncertainty in the retrieved source param-
587 eters are the observability of the monitoring network and model representa-
588 tiveness errors. It is noted that, quantification of the posterior uncertainties
589 in the retrieved source parameters is not obvious from the present renormal-
590 ization inversion methodology. However, these uncertainties can simply be
591 quantified by adding a controlled noise to the concentration measurements

592 and compute the source parameters with each noisy measurement. This ap-
593 proach is computationally expensive because it required the estimation of
594 source parameters for several times. However, in renormalization inversion
595 technique, it does not required to compute the weight function with each
596 noisy measurements because the computation of the weight function is inde-
597 pendent of the concentration measurements.

598 To quantify the uncertainties in source parameters in a 3-D space, 50 set of
599 noisy measurements (μ_i^{noisy}) are generated by adding a controlled 10% noise
600 in proportion to each concentration measurements μ_i , *i.e.* $\mu_i^{noisy} = \mu_i(1 + \alpha)$,
601 where α is a Gaussian distributed random number generated in $[-0.1, +0.1]$.
602 For these noisy measurements in each MUST trial, 50 source reconstruction
603 simulations are performed and the average and standard deviation (sd) of
604 these 50 estimated source parameters are calculated.

605 For all and non-zero measurements with 10% noise in each trial, the stan-
606 dard deviations (sd) of the estimated location error, height, and intensity are
607 presented in Table 2 and shown by error bar plots in Figures 3(a), (b)&(c).
608 With all measurements, minimum and maximum standard deviations in re-
609 trieved source height is observed in trial 7 (0.01 m) and trial 1 (7.91 m),
610 respectively (Figure 3(b), Table 2). On an average for all 20 trials, the es-
611 timated source height deviates by 0.80 m from their mean value. However,
612 with non-zero measurements with 10% noise, the averaged deviation (*i.e.* sd)
613 of estimated source height for all 20 trials is 1.46 m, with minimum 0.14 m
614 in trials 4, 14, & 15 and maximum 8.84 m in trial 20 (Figure 3(b), Table 2).

615 With all measurements, the averaged standard deviation in location error
616 (E_L) is 4.87 m with minimum 0.17 m in trial 20 and maximum 18.13 m in

trial 16 (Figure 3(a), Table 2). On other hand with non-zero measurements, the standard deviation of location error is minimum 0.21 m in trial 20 and maximum 24.28 m in trial 18, with an averaged 5.80 m of all trials. The release strength with all measurement varies by an averaged of $\approx 18\%$ from their mean value, with minimum variation in trials 1 and 20, and maximum standard deviation in trial 7 (Figure 3(c), Table 2). Whereas, with non-zero measurements, minimum and maximum standard deviations in retrieved release rate are observed in trial 20 and trial 7, respectively, with an average of $\approx 23\%$ from their mean value.

It is noted that with non-zero measurements, though the source parameters in a 3-D space are retrieved approximately similar to that estimated by taken all the measurements, the uncertainties in location error, intensity and release height increases slightly. It exhibits that the inclusion of the zero-concentration measurements has importance to reduce the uncertainty in the estimated continuous point source parameters in an urban region.

5.7. Comparison with Bayesian reconstruction results by Winiarek (2014)

Recently, Winiarek (2014) performed a source reconstruction study based on a stochastic Bayesian inversion approach to estimate the source parameters in 14 trials of the MUST field experiment. It is worth mentioning here that the present renormalization inversion approach is purely deterministic in nature and does not required any prior information about the point source parameters. However, the successfulness of a stochastic approach, like Bayesian, is dependent on a priori information about the source that generally is not known in reality. In addition, Winiarek (2014) considered only 14 trials; however, this study presented the source reconstruction results in 20

642 trials of the MUST field experiment.

643 With all measurements, the averaged Euclidean distance (E_L) between
644 the retrieved source location and the true source position with present deter-
645 ministic inversion methodology in these identical 14 trials is 15.5 m, which
646 is smaller than the location error $E_L = 22.3$ m, obtained with the stochastic
647 Bayesian approach by Winiarek (2014). For these 14 trials, the averaged es-
648 timated release rate with the present methodology is overpredicted within a
649 factor of 1.5 of the true source intensity which is slightly higher in comparison
650 to the Winiarek (2014) (*i.e.* the averaged $q_0/q_s = 1.2$). In present study, the
651 source intensity in $\approx 93\%$ (*i.e.* 13 trials) of these 14 trials is retrieved within
652 a factor of two; whereas, it was within in a factor of two for all the trials in
653 Winiarek (2014). In 50% of the these trials, the release height is estimated
654 within a factor of two with present study. However, in Winiarek (2014), the
655 estimated release height was within a factor of two in $\approx 43\%$ of these trials.

656 It is also noted that the application domain size which Winiarek (2014)
657 considered for the source reconstruction study is only slightly larger than the
658 geometry of MUST array and it is approximately equal to the inner domain
659 size taken in present study. However, in present study, source reconstruction
660 in each trial are applied to approximately four times larger domain than it.
661 Retrieval of a source in a smaller domain can have a higher probability of
662 its accurately estimation in comparison to the retrieval in a larger domain.
663 However, in present inversion methodology, it can be analyzed with the geo-
664 metrical representation of the visibility function, whether the well and poorly
665 seen regions extend to a larger area up to outer domain in each trial.

666 6. Conclusions

667 This study describes an atmospheric source reconstruction methodology
668 based on the *renormalization* inversion theory coupled with a building re-
669 solving CFD modelling approach to locate and quantify a continuous point
670 release in the urban environments. A salient feature of the methodology is
671 to address the problem of vertical structure (i.e. height of a source) in atmo-
672 spheric source reconstruction in three-dimensional space of an urban area.
673 The inversion methodology is purely deterministic in the sense that it does
674 not required any prior source information and utilizes only a finite number of
675 the ambient concentration measurements and a CFD model to determine the
676 source parameters (i.e. location, height, and strength) in an urban area. The
677 CFD model accounts the influences of buildings and other structures in com-
678 plex urban regions on flow-field and consequently on adjoint functions in a
679 3-dimensional space that required in the renormalization inversion technique.

680 The methodology is evaluated to retrieve the location, height, and strength
681 of a continuous point release in 20 trials of the MUST field experiment in
682 various atmospheric stability conditions varying from neutral to stable and
683 very stable. The retrieved source parameters in all the 20 trials are estimated
684 close to their true source. Different release heights of a point source located
685 at (i) ground level (ii) middle of the buildings (iii) two-thirds of the urban
686 height (iv) roof of the buildings, and (v) above the urban heights, at different
687 horizontal locations in the MUST urban domain are retrieved and analysed.
688 In 55% and 75% of the MUST trials, the source height is retrieved within a
689 factor of two and four, respectively. The averaged location error for all 20
690 trials is attained 14.54 m with minimum 3.58 m and maximum 34.55 m. In

691 $\approx 85\%$ of the trials, the source intensity is retrieved within in factor of two.
692 For all trials, the averaged estimated release rate with all measurements is
693 overpredicted within a factor of 1.48 of the true source intensity. The source
694 reconstruction for all the trials is also performed with non-zero measure-
695 ments only. It was observed that the use of all concentration measurements
696 instead of only non-zero essentially makes the small differences in quality of
697 the source reconstruction and gives a little additional information for better
698 constraining the source parameters.

699 A posteriori uncertainty analysis in the retrieved source parameters is
700 also carried out with respect to a controlled 10% noise in the concentration
701 measurements. It is shown that the standard deviation in the release height,
702 location error, and source intensity vary by 0.80 m, 4.87 m, and $\approx 18\%$,
703 respectively from their mean value for all 20 trials. The source reconstruction
704 results are also compared with an earlier study based on a stochastic Bayesian
705 approach for the identical 14 MUST trials, and it was shown that the present
706 methodology is relatively more efficient. Although the urban domain in the
707 present application was less than a kilometer, the methodology can also be
708 used for a larger domain as the CFD models can drive the representative
709 flow-field and dispersion in the larger urban domains. The application of the
710 source reconstruction methodology shows that combining the renormalization
711 inversion theory with a building resolving CFD modelling approach provides
712 an efficient and effective source determination tool in 3-dimensional space of
713 an urban region.

714 **Appendix A: Minimum weighted-norm solution**

715 By introducing the Lagrange multipliers $\boldsymbol{\lambda} \in \mathbb{R}^m$, an auxiliary function
 716 $\mathcal{L}(\mathbf{s}, \boldsymbol{\lambda})$ is formed as:

$$\mathcal{L}(\mathbf{s}, \boldsymbol{\lambda}) = \mathbf{s}^T \mathbf{W} \mathbf{s} + \boldsymbol{\lambda}^T (\boldsymbol{\mu} - \mathbf{A}_w \mathbf{W} \mathbf{s}) \quad (\text{A.1})$$

and solving $\nabla_{\mathbf{s}, \boldsymbol{\lambda}} \mathcal{L}(\mathbf{s}, \boldsymbol{\lambda}) = 0$, gives:

$$\nabla_{\mathbf{s}} \mathcal{L} = 2\mathbf{W} \mathbf{s} - \mathbf{W} \mathbf{A}_w^T \boldsymbol{\lambda} = 0 \quad (\text{A.2a})$$

$$\nabla_{\boldsymbol{\lambda}} \mathcal{L} = \boldsymbol{\mu} - \mathbf{A}_w \mathbf{W} \mathbf{s} = 0 \quad (\text{A.2b})$$

717 Eq. (A.2a) implies that $\mathbf{s} = \frac{1}{2} \mathbf{A}_w^T \boldsymbol{\lambda}$ and substituting it in Eq. (A.2b), one
 718 obtains $\boldsymbol{\lambda} = 2 (\mathbf{A}_w \mathbf{W} \mathbf{A}_w^T)^{-1} \boldsymbol{\mu} = 2 \mathbf{H}_w^{-1} \boldsymbol{\mu}$. It implies that the source estimate
 719 function $\mathbf{s}_w = \mathbf{A}_w^T \mathbf{H}_w^{-1} \boldsymbol{\mu}$.

720 **Acknowledgement**

721 The Mock Urban Setting Test (MUST) database is available at [https://must-](https://must-dpg.dpg.army.mil/)
 722 [dpg.dpg.army.mil/](https://must-dpg.dpg.army.mil/). The authors would like to thank the Defense Threat
 723 Reduction Agency (DTRA) for providing access to the MUST field exper-
 724 iment dataset. The authors gratefully acknowledge Fluidyn France for use
 725 of the CFD model fluidyn-PANACHE. A sincere thanks to Damien Joseph,
 726 Dr. Malo Le Guellec and Dr. Claude Souprayen, all from Fluidyn France,
 727 for discussions and helping in CFD simulation. The first author, Pramod
 728 Kumar, would also like to extend his sincerest thanks and appreciation to
 729 Dr. Jean-Pierre Issartel for fruitful discussion of the renormalization inver-
 730 sion theory and his encouragement. This work was supported by the RAPID
 731 project DISCARD (no. 132906009) funded by the French Defence Procure-
 732 ment Agency (DGA) and French Ministry of Industry.

733 **References**

- 734 Beljaars, A., Holtslag, A., 1991. Flux parameterization over land surfaces
735 for atmospheric models. *Journal of Applied Meteorology* 30 (3), 327–341.
736 URL [http://dx.doi.org/10.1175/1520-0450\(1991\)030<0327:FPOLSF>2.0.CO;2](http://dx.doi.org/10.1175/1520-0450(1991)030<0327:FPOLSF>2.0.CO;2)
- 737 Biltoft, C. A., 2001. Customer report for Mock Urban Setting Test. Tech.
738 rep., West Desert Test Center, U.S. Army Dugway Proving Ground, Dug-
739 way, Utah.
- 740 Bocquet, M., 2005. Reconstruction of an atmospheric tracer source using the
741 principle of maximum entropy. I: Theory. *Quarterly Journal of the Royal*
742 *Meteorological Society* 131 (610), 2191–2208.
743 URL <http://dx.doi.org/10.1256/qj.04.67>
- 744 Brown, M. J., 2004. Urban dispersion-challenges for fast response modeling.
745 In: *Fifth AMS Symposium on the Urban Environment*.
- 746 Chow, F. K., Kosovic, B., Chan, S., 2008. Source inversion for contaminant
747 plume dispersion in urban environments using building-resolving simula-
748 tions. *Journal of applied meteorology and climatology* 47 (6), 1553–1572.
749 URL <http://dx.doi.org/10.1175/2007JAMC1733.1>
- 750 Ferziger, J. H., Peric, M., 2002. *Computational Methods for Fluid Dynamics*.
751 Springer Berlin Heidelberg.
- 752 Fluidyn-PANACHE, 2010. User Manual. FLUIDYN France / TRANSOFT
753 International, version 4.0.7 Edition.

- 754 Gryning, S.-E., Batchvarova, E., Brummer, B., Jrgensen, H., Larsen, S., 2007.
 755 On the extension of the wind profile over homogeneous terrain beyond the
 756 surface boundary layer. *Boundary-Layer Meteorology* 124 (2), 251–268.
 757 URL <http://dx.doi.org/10.1007/s10546-007-9166-9>
- 758 Hanjalic, K., 2005. Turbulence and transport phenomena: Modelling and
 759 simulation. In: *Turbulence Modeling and Simulation (TMS) Workshop*.
 760 Technische Universitt Darmstadt.
- 761 Hanna, S. R., Hansen, O. R., Dharmavaram, S., 2004. FLACS CFD air
 762 quality model performance evaluation with kit fox, must, prairie grass,
 763 and EMU observations. *Atmospheric Environment* 38 (28), 4675–4687.
 764 URL <http://www.sciencedirect.com/science/article/pii/S1352231004005345>
- 765 Haupt, S. E., Young, G. S., Allen, C. T., 2006. Validation of a receptor-
 766 dispersion model coupled with a genetic algorithm using synthetic data.
 767 *Journal of applied meteorology and climatology* 45 (3), 476–490.
 768 URL <http://dx.doi.org/10.1175/JAM2359.1>
- 769 Hourdin, F., Talagrand, O., 2006. Eulerian backtracking of atmospheric trac-
 770 ers. I: Adjoint derivation and parametrization of subgrid-scale transport.
 771 *Quarterly Journal of the Royal Meteorological Society* 132 (615), 567–583.
 772 URL <http://dx.doi.org/10.1256/qj.03.198.A>
- 773 Issartel, J.-P., 2005. Emergence of a tracer source from air concentration
 774 measurements, a new strategy for linear assimilation. *Atmospheric Chem-
 775 istry and Physics* 5 (1), 249–273.
 776 URL <http://www.atmos-chem-phys.net/5/249/2005/>

777 Issartel, J.-P., Sharan, M., Modani, M., 2007. An inversion technique to
 778 retrieve the source of a tracer with an application to synthetic satellite
 779 measurements. *Proceedings of the Royal Society of London A: Mathemat-*
 780 *ical, Physical and Engineering Sciences* 463 (2087), 2863–2886.
 781 URL <http://rspa.royalsocietypublishing.org/content/463/2087/2863.abstract>

782 Keats, A., Yee, E., Lien, F.-S., 2007. Bayesian inference for source determi-
 783 nation with applications to a complex urban environment. *Atmospheric*
 784 *Environment* 41 (3), 465 – 479.
 785 URL <http://www.sciencedirect.com/science/article/pii/S1352231006008703>

786 Kovalets, I. V., Andronopoulos, S., Venetsanos, A. G., Bartzis, J. G.,
 787 2011. Identification of strength and location of stationary point source
 788 of atmospheric pollutant in urban conditions using computational fluid
 789 dynamics model. *Mathematics and Computers in Simulation* 82 (2), 244
 790 – 257.
 791 URL <http://www.sciencedirect.com/science/article/pii/S0378475411001686>

792 Kumar, P., Feiz, A.-A., Ngae, P., Singh, S. K., Issartel, J.-P., 2015a. CFD
 793 simulation of short-range plume dispersion from a point release in an
 794 urban like environment. *Atmospheric Environment* 122, 645 – 656.
 795 URL <http://www.sciencedirect.com/science/article/pii/S1352231015304465>

796 Kumar, P., Feiz, A.-A., Singh, S. K., Ngae, P., Turbelin, G., 2015b. Recon-
 797 struction of an atmospheric tracer source in an urban-like environment.
 798 *Journal of Geophysical Research: Atmospheres* 120 (24), 12589–12604,
 799 2015JD024110.
 800 URL <http://dx.doi.org/10.1002/2015JD024110>

- 801 Launder, B., 2004. Turbulence modelling of buoyancy-affected flows. In: Sin-
802 gapore Turbulence Colloquium.
- 803 Luhar, A. K., Etheridge, D. M., Leuning, R., Loh, Z. M., Jenkins, C. R.,
804 Yee, E., 2014. Locating and quantifying greenhouse gas emissions at a ge-
805 ological CO₂ storage site using atmospheric modeling and measurements.
806 Journal of Geophysical Research: Atmospheres 119 (18), 10,959–10,979,
807 2014JD021880.
808 URL <http://dx.doi.org/10.1002/2014JD021880>
- 809 Marchuk, G. I., 1995. Adjoint Equations and Analysis of Complex Systems.
810 Springer Netherlands.
- 811 Penenko, V., Baklanov, A., Tsvetova, E., 2002. Methods of sensitivity
812 theory and inverse modeling for estimation of source parameters. Future
813 Generation Computer Systems 18 (5), 661 – 671, {ICCS2001}.
814 URL <http://www.sciencedirect.com/science/article/pii/S0167739X02000316>
- 815 Pudykiewicz, J. A., 1998. Application of adjoint tracer transport equations
816 for evaluating source parameters. Atmospheric Environment 32 (17),
817 3039–3050.
818 URL <http://www.sciencedirect.com/science/article/pii/S1352231097004809>
- 819 Saide, P., Bocquet, M., Osses, A., Gallardo, L., 2011. Constraining surface
820 emissions of air pollutants using inverse modelling: method intercompari-
821 son and a new two-step two-scale regularization approach. Tellus B 63 (3),
822 360–370.
823 URL <http://dx.doi.org/10.1111/j.1600-0889.2011.00529.x>

- 824 Sharan, M., Issartel, J.-P., Singh, S. K., Kumar, P., 2009. An inversion
825 technique for the retrieval of single-point emissions from atmospheric
826 concentration measurements. *Proceedings of the Royal Society of London*
827 *A: Mathematical, Physical and Engineering Sciences* 465, 2069–2088.
828 URL <http://rspa.royalsocietypublishing.org/content/early/2009/04/09/rspa.2008.0>
- 829 Sharan, M., Kumar, P., 2010. Estimation of upper bounds for the appli-
830 cability of non-linear similarity functions for non-dimensional wind and
831 temperature profiles in the surface layer in very stable conditions. *Pro-*
832 *ceedings of the Royal Society of London A: Mathematical, Physical and*
833 *Engineering Sciences* 467 (2126), 473–494.
- 834 Singh, S. K., Sharan, M., Singh, A. K., 2015a. Reconstructing height of
835 an unknown point release using least-squares data assimilation. *Quarterly*
836 *Journal of the Royal Meteorological Society* 141 (689), 1376–1388.
837 URL <http://dx.doi.org/10.1002/qj.2446>
- 838 Singh, S. K., Turbelin, G., Issartel, J.-P., Kumar, P., Feiz, A. A., 2015b.
839 Reconstruction of an atmospheric tracer source in fusion field trials: Ana-
840 lyzing resolution features. *Journal of Geophysical Research: Atmospheres*
841 120 (12), 6192–6206, 2015JD023099.
842 URL <http://dx.doi.org/10.1002/2015JD023099>
- 843 Turbelin, G., Singh, S. K., Issartel, J.-P., 2014. Reconstructing source terms
844 from atmospheric concentration measurements: Optimality analysis of an
845 inversion technique. *Journal of Advances in Modeling Earth Systems* 6 (4),
846 1244–1255.
847 URL <http://dx.doi.org/10.1002/2014MS000385>

- 848 Van Doormaal, J. P., Raithby, G. D., 1984. Enhancements of the simple
849 method for predicting incompressible fluid flows. *Numerical Heat Transfer*
850 7 (2), 147–163.
851 URL <http://dx.doi.org/10.1080/01495728408961817>
- 852 Winiarek, V., 2014. Dispersion atmosphérique et modélisation inverse pour
853 la reconstruction de sources accidentelles de polluants. Ph.D. thesis, Uni-
854 versité Paris-Est.
855 URL <https://pastel.archives-ouvertes.fr/tel-01004505>
- 856 Winiarek, V., Bocquet, M., Saunier, O., Mathieu, A., 2012. Estimation of
857 errors in the inverse modeling of accidental release of atmospheric pollu-
858 tant: Application to the reconstruction of the cesium-137 and iodine-131
859 source terms from the fukushima daiichi power plant. *Journal of Geophys-*
860 *ical Research: Atmospheres* 117 (D5), D05122, d05122.
861 URL <http://dx.doi.org/10.1029/2011JD016932>
- 862 Yang, Y., Gu, M., Chen, S., Jin, X., 2009. New inflow boundary conditions
863 for modelling the neutral equilibrium atmospheric boundary layer in
864 computational wind engineering. *Journal of Wind Engineering and*
865 *Industrial Aerodynamics* 97 (2), 88–95.
866 URL <http://www.sciencedirect.com/science/article/pii/S0167610508001815>
- 867 Yee, E., Bilitoft, C., 2004. Concentration fluctuation measurements in a plume
868 dispersing through a regular array of obstacles. *Boundary-Layer Meteorol-*
869 *ogy* 111 (3), 363–415.
870 URL <http://dx.doi.org/10.1023/B%3ABOUN.0000016496.83909.ee>

871 Yee, E., Hoffman, I., Ungar, K., 2014. Bayesian inference for source recon-
872 struction: A real-world application. International Scholarly Research No-
873 tices 2014, 1–12.
874 URL <http://dx.doi.org/10.1155/2014/507634>

875 List of Tables

- 876 1 The selected 20 trials of the MUST field experiments with
877 source, meteorological, and turbulence parameters (Biltoft,
878 2001; Yee and Biltoft, 2004). z_s , t_s , and q_s are respectively
879 the effective source height, duration, and release rate. S_{04}
880 and α_{04} are the wind speed and direction respectively at a 4
881 m level of mast S. The Obukhov length (L), friction velocity
882 (u_*), and turbulent kinetic energy (k) are at 4 m level of tower
883 T. The Trial No. 1-20 are assigned here for just continuation
884 and simplicity and these do not correspond to the same trial
885 no. as assigned for a Trial name in the MUST experiment. . . 42
- 886 2 Source reconstruction results for all 20 trials of MUST field
887 experiment by considering all (i.e. $m = 40$) and non-zero mea-
888 surements in each trial. Here, m is the no. of measurements
889 considered for source retrieval in each trial. q_s and q_0 repre-
890 sent the true and estimated release rates, respectively. z_s and
891 z_0 are respectively the true and estimated source height. The
892 location error (E_L) represents the Euclidian distance of the
893 retrieved source location from the true position. $E_q = q_0/q_s$ is
894 a ratio of the retrieved and the true release rates in each trial. 43

895 List of Figures

896	1	Layout of the MUST urban geometry showing 120 containers,	
897		source, and receptor locations. The black circles denote the	
898		position of receptors. The stars denote the source locations -	
899		only one was operational in a given trial.	44
900	2	Isopleths of the weight functions $w(\mathbf{x})$ (m^{-2}) (in panel a) and	
901		the normalized source estimate $s_w^n(\mathbf{x}) = s_w(\mathbf{x})/\max(\mathbf{s}_w)$ (in	
902		panel b) in a horizontal plane corresponding to the estimated	
903		effective source height (z_0) in trials 3, 9, 11, 15, and 16, with	
904		all and non-zero concentration measurements. The black and	
905		white filled circles in panels (b) show the true and estimated	
906		source locations, respectively.	45
907	3	Bar plots for (a) Location error (E_L), (b) estimated effective	
908		source height (z_0), and (c) source intensity ratios ($E_q = q_0/q_s$).	
909		The corresponding uncertainties (standard deviation) are rep-	
910		resented by the errorbars.	46

Table 1: The selected 20 trials of the MUST field experiments with source, meteorological, and turbulence parameters (Biltoft, 2001; Yee and Biltoft, 2004). z_s , t_s , and q_s are respectively the effective source height, duration, and release rate. S_{04} and α_{04} are the wind speed and direction respectively at a 4 m level of mast S. The Obukhov length (L), friction velocity (u_*), and turbulent kinetic energy (k) are at 4 m level of tower T. The Trial No. 1-20 are assigned here for just continuation and simplicity and these do not correspond to the same trial no. as assigned for a Trial name in the MUST experiment.

Trial No.	Trial Name (JJJhhmm)	q_s (l/min)	t_s (min)	z_s (m)	S_{04} (m/s)	α_{04} (deg)	u_* (m/s)	L (m)	k (m^2s^{-2})
1	2640138	175	21	0.15	2.35	17	0.26	91	0.359
2	2640246	200	15	0.15	2.01	30	0.25	62	0.306
3	2671852	200	22	0.15	3.06	-49	0.32	330	0.436
4	2671934	200	15	1.8	1.63	-48	0.08	5.8	0.148
5	2672033	200	15	1.8	2.69	-26	0.17	4.8	0.251
6	2672101	200	14	0.15	1.89	-10	0.16	7.7	0.218
7	2672150	200	16	0.15	2.30	36	0.35	150	0.409
8	2672213	200	15	1.8	2.68	30	0.35	150	0.428
9	2672235	200	15	2.6	2.32	36	0.26	48	0.387
10	2672303	200	19	1.8	2.56	17	0.25	74	0.367
11	2681829	225	15	1.8	7.93	-41	1.10	28000	1.46
12	2681849	225	16	0.15	7.26	-50	0.76	2500	0.877
13	2682256	225	15	0.15	5.02	-42	0.66	240	0.877
14	2682320	225	15	2.6	4.55	-39	0.50	170	0.718
15	2682353	225	15	5.2	4.49	-47	0.44	120	0.727
16	2692054	225	22	1.3	3.34	39	0.36	170	0.362
17	2692131	225	17	1.3	4.00	39	0.42	220	0.582
18	2692157	225	15	2.6	2.98	43	0.39	130	0.505
19	2692223	225	15	1.3	2.63	26	0.35	120	0.484
20	2692250	225	17	1.3	3.38	36	0.37	130	0.537

Table 2: Source reconstruction results for all 20 trials of MUST field experiment by considering all (i.e. $m = 40$) and non-zero measurements in each trial. Here, m is the no. of measurements considered for source retrieval in each trial. q_s and q_0 represent the true and estimated release rates, respectively. z_s and z_0 are respectively the true and estimated source height. The location error (E_L) represents the Euclidian distance of the retrieved source location from the true position. $E_q = q_0/q_s$ is a ratio of the retrieved and the true release rates in each trial.

Trial No.	Trial Name (JJJhhmm)	q_s (l/min)	z_s (m)	All measurements				non-zero measurements				
				q_0 (l/min)	z_0 (m)	E_L (m)	E_q	m	q_0 (l/min)	z_0 (m)	E_L (m)	E_q
1	2640138	175.	0.15	356.93	2.38±7.91	12.33± 0.99	2.04±0.03	34	356.96	2.38±5.59	12.33± 0.94	2.04±0.04
2	2640246	200.	0.15	900.58	3.38±0.81	30.57±16.06	4.50±0.33	28	899.51	3.38±0.60	30.57±11.92	4.50±0.24
3	2671852	200.	0.15	117.51	2.63±0.26	21.80± 1.24	0.59±0.16	30	117.38	2.63±0.22	21.80± 1.10	0.59±0.13
4	2671934	200.	1.80	258.55	2.88±0.13	17.20± 2.74	1.29±0.21	31	258.97	2.88±0.14	17.20± 3.07	1.29±0.23
5	2672033	200.	1.80	161.46	0.38±0.89	13.80± 0.88	0.81±0.48	37	161.46	0.38±0.89	13.80± 0.88	0.81±0.48
6	2672101	200.	0.15	485.40	2.13±0.43	8.83± 1.19	2.43±0.10	40	485.40	2.13±0.43	8.83± 1.19	2.43±0.10
7	2672150	200.	0.15	81.24	0.13±0.01	12.44± 4.44	0.41±0.57	30	90.98	0.13±0.19	11.69± 8.95	0.45±1.19
8	2672213	200.	1.80	417.61	0.38±0.20	17.36± 0.69	2.09±0.06	30	432.56	0.13±1.85	18.66±14.88	2.16±0.42
9	2672235	200.	2.60	358.79	3.63±0.43	5.30± 2.63	1.79±0.19	31	367.49	3.63±5.59	4.30± 1.11	1.84±0.09
10	2672303	200.	1.80	221.49	1.13±0.39	11.32± 2.07	1.11±0.09	40	221.49	1.13±0.39	11.32± 2.07	1.11±0.09
11	2681829	225.	1.80	325.10	2.13±0.62	11.82± 9.83	1.44±0.18	30	323.96	2.13±0.65	11.82±10.87	1.44±0.19
12	2681849	225.	0.15	192.62	0.13±0.38	5.43± 4.65	0.86±0.11	27	192.03	0.13±0.38	5.43± 4.84	0.85±0.12
13	2682256	225.	0.15	243.48	1.38±0.66	6.72± 2.05	1.08±0.16	33	243.47	1.38±0.81	6.72± 1.74	1.08±0.14
14	2682320	225.	2.60	335.68	4.13±0.16	6.90± 1.88	1.49±0.08	29	335.90	4.13±0.14	6.90± 2.02	1.49±0.07
15	2682353	225.	5.20	306.12	4.38±0.30	4.22± 1.12	1.36±0.07	25	285.57	4.38±0.14	2.96± 1.12	1.27±0.05
16	2692054	225.	1.30	408.16	3.63±0.44	3.58±18.13	1.81±0.22	26	435.45	3.88±0.40	3.58± 6.95	1.94±0.10
17	2692131	225.	1.30	127.76	4.38±0.42	28.71± 5.00	0.57±0.16	31	127.15	4.38±0.37	28.71± 5.35	0.57±0.17
18	2692157	225.	2.60	321.87	4.13±0.45	12.33±12.02	1.43±0.27	33	320.75	4.13±0.83	12.33±24.29	1.43±0.54
19	2692223	225.	1.30	392.83	1.13±0.71	25.66± 9.59	1.75±0.14	35	391.94	1.13±0.71	25.66±12.64	1.74±0.18
20	2692250	225.	1.30	160.26	1.38±0.17	34.55± 0.17	0.71±0.03	31	163.64	0.13±8.84	35.29± 0.21	0.73±0.03

Figure 1: Layout of the MUST urban geometry showing 120 containers, source, and receptor locations. The black circles denote the position of receptors. The stars denote the source locations - only one was operational in a given trial.

Figure 2: Isopleths of the weight functions $w(\mathbf{x})$ (m^{-2}) (in panel a) and the normalized source estimate $s_w^n(\mathbf{x}) = s_w(\mathbf{x})/\max(\mathbf{s}_w)$ (in panel b) in a horizontal plane corresponding to the estimated effective source height (z_0) in trials 3, 9, 11, 15, and 16, with all and non-zero concentration measurements. The black and white filled circles in panels (b) show the true and estimated source locations, respectively.

Figure 3: Bar plots for (a) Location error (E_L), (b) estimated effective source height (z_0), and (c) source intensity ratios ($E_q = q_0/q_s$). The corresponding uncertainties (standard deviation) are represented by the errorbars.