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UNCERTAINTY ESTIMATION IN THE RECONSTRUCTION OF ATMOSPHERIC TRACER SOURCE EMISSIONS

Sarvesh Kumar Singh, Gregory Turbelin, Pramod Kumar, Raj Rani, Amir-Ali Feiz, Pierre Ngae

LMEE, Université d'Evry-Val d'Essonne, 40 Rue du Pelvoux, 91020 Evry Cedex

Abstract: In an inversion procedure, the interest is not only to obtain an estimate of the unknown parameters but also to determine the uncertainty involved in their estimation. The study proposes advancement within the framework of an inversion technique, called *Renormalization*, to characterize the uncertainties in a point source reconstruction. The novelty stems from the fact that the inherent uncertainties in the retrieved parameters are directly identifiable from the shape and features of the a posteriori source estimate. The uncertainty estimates are illustrated in point source reconstruction using the concentration measurements from field experiments, known as Fusion Field Trials 2007 (FFT07) at Dugway Proving Ground, Utah.

Key words: *FFT07, inverse problem, renormalization, source identification, uncertainty.*

INTRODUCTION

Fast growing industrialization and urbanization have posed significant risk towards the human environment and associated ecological systems. Any dispersion event caused intentionally or accidentally may lead fatal mortality in the environment. The notable examples can be seen in the past as, Bhopal gas leakage (December 2, 1984, India), Chernobyl disaster (April 26, 1986, Ukraine), Fukushima nuclear accident (March 11, 2011, Japan) etc. These examples raise the issues regarding the improvement of the emergency preparedness and national security which eventually require fast and preliminary information about the origin and strength of unknown releases caused into the atmosphere. The interest is not only to obtain an estimate but also to determine the uncertainty involved in their estimation.

The study highlights an inversion technique, called "*Renormalization*" (Issartel et al., 2007), recently proposed for the identification of a point release. The technique has been shown efficient in retrieving the origin and strength of a point release requiring minimal a priori information, however, a procedure for determining the uncertainty involved in the parametric estimates has not been developed so far. Thus, the objective here is to propose a methodology for determining the uncertainty involved in the retrieved point release parameters (mainly, location and strength).

Uncertainty estimation is mainly an analysis of the information gained by the measurements over a priori information about the unknown release. The inversion technique lead to a conditional estimate, often called a posteriori, which needs to be inspected in several directions in order to determine the uncertainties associated with this conditional estimate. In a point source reconstruction, maximum of a posteriori provides the location of the point release. Thus, the shape or a distribution of the maxima region may provide an indication of the uncertainties involved. The estimation is said to be well resolved when the source estimate is sharply peaked. These features are explored and quantified in this study and the uncertainty estimation methodology is evaluated with real data taken from Fusion Field Trials 2007 (FFT07) (Storwald, 2007) conducted at Dugway Proving Ground, Utah, USA.

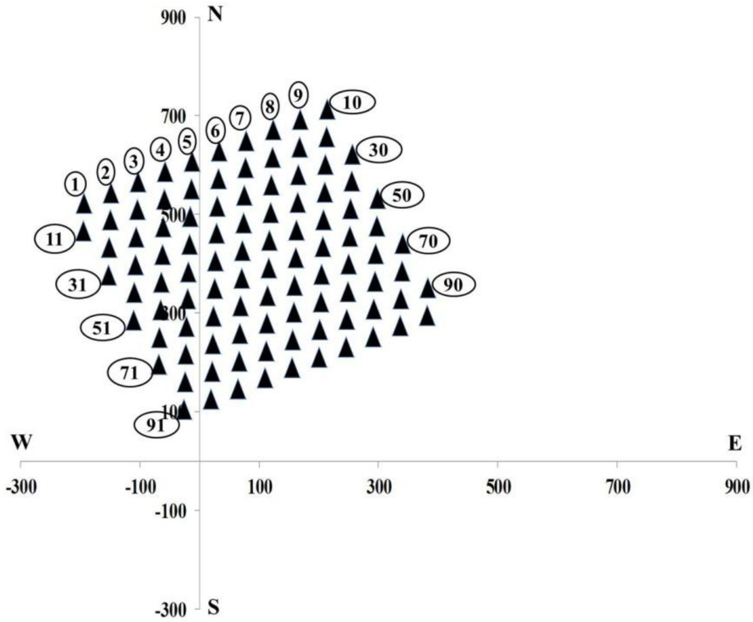

Figure 1. Layout of the FFT07 experiment. The triangles denote detectors. Their index number are highlighted in the circles.

The FFT07 experiment consist of 100 digital Photoionization Detectors (digiPID) arranged in a rectangular staggered array (10 rows and 10 columns) in an area 475 m × 450 m. The wind flows from south-east to north-west direction. To take an advantage of the prevailing wind direction, the detector's grid was rotated 25° towards west. The spacing between subsequent rows and columns were 50 m. A tracer propylene was released from a height of 2 m continuously for an approximate duration of 10 min. The concentration measurements were collected at a height of 2 m. The release location varies in each trial. The meteorological measurements (wind, temperature, stability etc.,) are taken at 4 m level from a 32 m meteorological tower located at the centre of the grid.

METHODOLOGY

The inversion technique is described here for point source identification in a least-square framework. For simplicity, the release is assumed continuous and ground level. Accordingly, the identification of a point release refers to the estimation of its location and strength. The source-receptor relationship is described here with the use of an adjoint modelling framework. In discrete notations, a source-receptor relationship is denoted as (Pudykiewicz, 1998),

$$\boldsymbol{\mu} = \mathbf{A}\mathbf{s} + \boldsymbol{\varepsilon} \tag{1}$$

in which $\boldsymbol{\mu}$ is the measured concentration vector of dimension *m*, $\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_N]$ is the sensitivity matrix of dimension $m \times N$, $\mathbf{s}$ is the source vector of dimension N and $\boldsymbol{\varepsilon}$ denotes measurement error vector of dimension *m*. Assuming a priori that the nature of the release is point type, the source vector $\mathbf{s}$ is parameterized as $\mathbf{s} = q\delta(x - x_o)(y - y_o)$ where q is the release strength and $\mathbf{x}_o = (x_o, y_o)$ is the ground level release location coordinates. Using the definition of a point source, equation (1) can be reformulated as (Sharan et al., 2009),

$$\boldsymbol{\mu} = q\mathbf{a}(\mathbf{x}_o) + \boldsymbol{\varepsilon} \tag{2}$$

Issartel et al. (2007) have shown that the sensitivity matrix is associated with peaks at the sensitivity vectors coinciding with the cells containing measurements due to the diffusive nature of the transport and strong concentration gradient around the measurement cells. To deal with this, a diagonal weight matrix $\mathbf{W} = [w_{ij}]$ of dimension $N \times N$ is proposed (it satisfies properties, $trace(\mathbf{W}) = m$ and $\mathbf{a}_w^{\mathrm{T}}(\mathbf{x})\mathbf{H}_w^{-1}\mathbf{a}_w(\mathbf{x}) = 1$) in such a way it normalizes the sensitivity vectors as, $\mathbf{a}_w(\mathbf{x}_i) = \mathbf{a}(\mathbf{x}_i)/w_{ii}$ (Issartel et al., 2007; Singh et al., 2015). Accordingly, the equation (2) is modified as,

$$\boldsymbol{\mu} = qw(\mathbf{x}_o)\mathbf{a}_w(\mathbf{x}_o) + \boldsymbol{\varepsilon} \tag{3}$$

Least-squares estimation of release parameters

To estimate the release parameters $\mathbf{x}_o$ and q, a least-squares cost function is formulated from equation (3) as $J = \frac{1}{2}\boldsymbol{\varepsilon}^{\mathrm{T}}\mathbf{H}_w^{-1}\boldsymbol{\varepsilon}$. In this, matrix $\mathbf{H}_w = \mathbf{A}_w\mathbf{W}\mathbf{A}_w^{\mathrm{T}}$ is regarded as measurement covariance matrix since it measures for the dispersion in the sensitivity vectors which are linear to the measurements. The minimization of J is performed, first, with respect to q and then for $\mathbf{x}$. In the first step, minimization of J with respect to q leads to a critical estimate by equating $\partial J / \partial q = 0$ as,

$$\hat{q} = \frac{\mathbf{a}_w^{\mathrm{T}}(\mathbf{x})\mathbf{H}_w^{-1}\boldsymbol{\mu}}{w(\mathbf{x})} \tag{4}$$

From equation (4), the cost function J is simplified as, $J = \frac{1}{2}\left(\boldsymbol{\mu}^{\mathrm{T}}\mathbf{H}_w^{-1}\boldsymbol{\mu} - \left(\mathbf{a}_w^{\mathrm{T}}(\mathbf{x})\mathbf{H}_w^{-1}\boldsymbol{\mu}\right)^2\right)$. Thus, minimization of J is equivalent to the maximization of $S'(\mathbf{x}) = \mathbf{a}_w^{\mathrm{T}}(\mathbf{x})\mathbf{H}_w^{-1}\boldsymbol{\mu}$. By implementing this analogy on a discrete domain, the location of the point source can be identified by searching exhaustively the maximum of the estimate S' in the domain. Once the release location $\hat{\mathbf{x}}_o$ is retrieved, its strength $\hat{q}$ can be derived from equation (4).

A posteriori estimation of variance in $\hat{q}$ and confidence bounds

A posteriori estimation of variance in q i.e., $\mathrm{var}(\hat{q})$ is based on the fact that $\mathbf{H}_w$ is proportional to the measurement dispersion matrix. Thus, $E\left[\boldsymbol{\mu}\boldsymbol{\mu}^{\mathrm{T}}\right] = \sigma\mathbf{H}_w$, where σ is the proportionality constant. Now, $\mathrm{var}(\hat{q})$ can be given as,

$$\mathrm{var}(\hat{q}) = \mathrm{var}\left(\frac{\mathbf{a}_w^{\mathrm{T}}(\hat{\mathbf{x}}_o)\mathbf{H}_w^{-1}\boldsymbol{\mu}}{w(\hat{\mathbf{x}}_o)}\right) = \frac{\mathbf{a}_w^{\mathrm{T}}(\hat{\mathbf{x}}_o)\mathbf{H}_w^{-1}\,\mathrm{var}(\boldsymbol{\mu})\mathbf{H}_w^{-1}\mathbf{a}_w(\hat{\mathbf{x}}_o)}{w^2(\hat{\mathbf{x}}_o)} < \frac{\mathbf{a}_w^{\mathrm{T}}(\hat{\mathbf{x}}_o)\mathbf{H}_w^{-1}E\left[\boldsymbol{\mu}\boldsymbol{\mu}^{\mathrm{T}}\right]\mathbf{H}_w^{-1}\mathbf{a}_w(\hat{\mathbf{x}}_o)}{w^2(\hat{\mathbf{x}}_o)} \tag{5}$$

$$\mathrm{var}(\hat{q}) < \frac{\sigma}{w^2(\hat{\mathbf{x}}_o)} \tag{6}$$

From equation (6), an upper bound of the $\mathrm{var}(\hat{q})$ can be determined by estimating the constant σ. An estimate $\hat{\sigma}$ can be obtained from the residuals since $E\left[\hat{\boldsymbol{\varepsilon}}\hat{\boldsymbol{\varepsilon}}^{\mathrm{T}}\right] = \sigma\mathbf{H}_w\left[\mathbf{I}_m - \mathbf{a}_w(\hat{\mathbf{x}}_o)\mathbf{a}_w^{\mathrm{T}}(\hat{\mathbf{x}}_o)\mathbf{H}_w^{-1}\right]$ where $\hat{\boldsymbol{\varepsilon}} = \boldsymbol{\mu} - \hat{q}w(\hat{\mathbf{x}}_o)\mathbf{a}_w(\hat{\mathbf{x}}_o)$ and $\mathbf{I}_m$ is $m \times m$ identity matrix. By using trace operator and simple linear algebra, it is derived as, $\hat{\sigma} = \frac{\hat{\boldsymbol{\varepsilon}}\mathbf{H}_w^{-1}\hat{\boldsymbol{\varepsilon}}^{\mathrm{T}}}{m-1}$.

The true variance of the release strength is not known and, under Gaussian assumptions, $\mathrm{var}(\hat{q})$ can be considered as an approximation to the standard error in $\hat{q}$. Hence, an upper bound estimate for $\mathrm{var}(\hat{q})$ can be utilized to construct the 95% confidence interval for $\hat{q}$ and $\hat{\mathbf{x}}_o$ using student t-distribution as,

$$P\left(-t_{m-1,\,0.975} < \frac{q - \hat{q}}{\hat{\sigma} / w^2(\hat{\mathbf{x}}_o)} < t_{m-1,\,0.975}\right) = 0.95 \tag{7}$$

The 95% confidence region for retrieved point source location can be determined as,

$$P\left(-t_{m-1,\,0.975} < \frac{S'(\mathbf{x}) - \hat{S}'(\hat{\mathbf{x}}_o)}{\hat{\sigma}} < t_{m-1,\,0.975}\right) = 0.95\,. \tag{8}$$

EVALUATION AND RESULTS

The proposed methodology is evaluated using non-zero real measurements of Trial#7 from FFT07 dispersion experiment. For a numerical implementation of the methodology, a domain of size 1200 m × 1200 m is chosen and discretized into 399 × 399 cells (figure 1). The true source location is at cell (200, 200) and true strength was 5.5 g s^{-1}. The important step of the inversion algorithm is the computation of sensitivity matrix **A** and weight matrix **W**. The sensitivity elements are derived from the solution of the adjoint dispersion model governing the transport and dispersion of a release tracer from a continuous, non-reactive tracer and ground level source. An analytical dispersion model developed by Sharan et al. (1996) is established in the adjoint mode by inverting the wind direction and replacing the source location by the measurement cell. This is possible since advection and diffusion operators are taken linear, wind is steady and diffusion is self-adjoint. The weight matrix is computed by an algorithm given in Issartel et al. (2007).

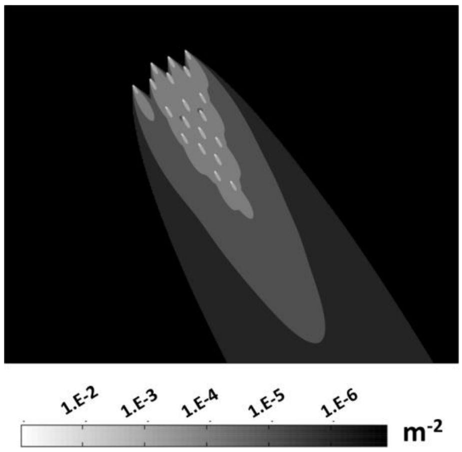

Figure 2. Distribution of weights in the domain.

The distribution of weights (figure 2) describes a priori information about unknown emissions apparent to the monitoring network. The weights are maximum at the measurement cells and decreasing further as one move away in upwind direction of the monitoring network. Figure (3) describes the normalized distribution of retrieved source $S'(\mathbf{x})$ in which the maxima region is associated with the informative source region.

The maxima region contain an extended branch in the upwind direction which arises mainly due to lack of visibility by the monitoring network in these regions and thus, corresponds to the poor model resolution. From the inversion technique, the maximum of $S'(\mathbf{x})$ will provide the point release location. With real data, the source location is retrieved very close to the true release location. The location error (Euclidean distance between the true and retrieved release location) is observed as 3 m. The source strength is also retrieved (as 6.98 g s^{-1}) within a factor of 1.3. The retrieval errors are mainly due to the model representation errors.

The 95% confidence bounds are derived for the source location and strength and a confidence region for the retrieved source location is highlighted in figure (3). The confidence region is observed similar to an ellipse elongated in the wind direction. The uncertainty in the location error is determined by measuring the length of the major axis. The 95% confidence interval is obtained for the location error (in meters) as [0, 53] m and for strength as [4.9, 9] g s^{-1}. This implies that the release parameters are significantly sensitive to the uncertainty in the measurements and model. For a comparison, the confidence estimates are also derived by using a Bootstrap resampling procedure. With bootstrap procedure, the 95% confidence interval for location error is observed as [0, 80] m while for strength, it is [2.2, 14.3] g s^{-1}. The present estimates are observed under-predicted (within a factor of 1.5) in comparison to bootstrap which may not be surprising since $\mathbf{H}_w$ is only an approximation to the measurement covariance based on overlapping of the sensitivity vectors. It is possible that the cross-correlations between the measurements are not being accounted properly or under/over-predicted which results into such deviations from actual uncertainty. However, figure (3) shows that the confidence region with present methodology is found comparable to the bootstrap estimates.

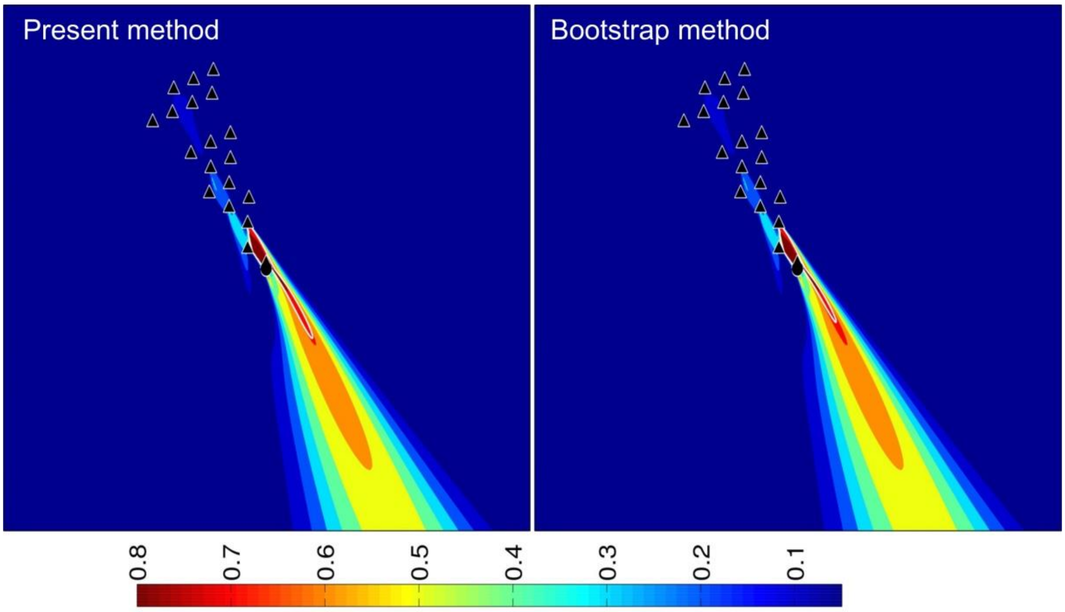

Figure 3. Isopleths of $\dfrac{S'(\mathbf{x})}{\max(S'(\mathbf{x}))}$. The black and white circles show true and retrieved source, respectively. The confidence region for point source location is shown by white line.

CONCLUSION

The study presents an uncertainty estimation methodology for point source reconstruction in the framework of renormalization inversion technique. The methodology is evaluated with real data taken from trial# 7 in FFT07 experiment. It is observed that the release parameters are retrieved close to their true values. In spite of their closeness towards the true parameters, their uncertainty is found to be large. The methodology is computationally efficient in determining uncertainty in comparison to the other methods based on sampling procedure or Hessian since it does not require any sampling or derivative information. However, a further investigation with several datasets is required to highlight the efficiency and accuracy of this methodology.

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