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An Inversion Method to Backtrack Source Parameters and Associated Concentration Field for an Inert Gas Release in Urban Environments

by Yansen Wang

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Yansen Wang
Computational and Information Sciences Directorate, ARL

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14. ABSTRACT This document describes a prototype of an inversion method to reconstruct the unknown atmospheric release parameters, including the release location and strength, and associated concentration field. The inversion method is based on the analysis of the data collected from wind, chemical/biological sensors. A combined process of backward trajectory and Bayesian inference is used for the inversion. The retrieved atmospheric release location and strength by this method are the optimal estimations of the physical parameters. A simple test case is used to demonstrate the accuracy and application of the inversion method.				
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1. Objective

The objective of this research is to develop an inversion method to reconstruct the unknown atmospheric release parameters, including the release location and strength and associated concentration field, in an event of a terrorist attack. The inversion method is based on the analysis of the data collected from wind, chemical/biological (CB) sensors. The retrieved atmospheric release location and strength by this method should be the optimal estimations of the physical parameters. The reconstructed source characteristics and concentration field are useful information for force protection and emergency responses such as delivering medical treatments, disinfecting affected areas, and analyzing forensic evidence. The retrieved source characteristics are also the necessary data for forecasting CB transport.

2. Approach

This source reconstruction system integrates the backward puff trajectory and the Bayesian inference methods to retrieve the physical parameters. The system consists of the data from CB detection sensors and the wind field from a diagnostic wind model, the three-dimensional (3-D) wind field (3-DWF) (*1*). The 3-DWF interpolates a limited number of wind observations to the computational domain using the mass conservation as a constraint. A backward puff trajectory using the mean wind field from the 3-DWF is computed to trace back to an approximated area of release location. The improbable release area is quickly eliminated from the backward trajectory. This step is also used as a detection step to ensure that the release location is in the computational domain. After the backward trajectory computation, the CB sensor and wind field data are integrated together to find the exact release location and strength using a dynamical Bayesian inference theory. The Bayesian theory gives a maximum likelihood estimate of the release parameters. During the Bayesian process, a forward model dispersion model, named the Lagrangian Gaussian puff model (LGPM) (*2, 3*), is applied to compute the concentration at each iterative cycle. The values of concentration from CB sensors and the LGPM model are compared and used to compute a likelihood function. The converged state from the iteration is the maximum likelihood estimate of the source parameters.

The backward puff trajectory uses the mean wind field computed from the 3-DWF model and parameterized turbulence. The velocity of a puff centroid at $(\boldsymbol{x_p}, t)$ in a forward time frame can be computed as $\boldsymbol{u} = d\boldsymbol{x_p}/dt$. The backward trajectory can be computed using a time coordinate $t_b = T_0 - t$, where T_0 is an arbitrary starting time. The velocity $\boldsymbol{u_b}$ of the puff in the backward time frame is as follows:

$$\boldsymbol{u_b} = d\boldsymbol{x_p}/d(T_0 - t) = -d\boldsymbol{x_p}/dt. \tag{1}$$

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By integrating equation 1 backward with respect to time, a backward puff trajectory line can be computed. In order to take care of the situation of an unsteady wind field, the wind field needs to be frequently updated from the 3-DWF and observations.

The puff turbulence spread parameters, σ_h and σ_z, can be estimated from the distance between the sensors with maximum and minimum readings. This method requires that multiple sensors are available for CB detection. In general CB detection practice, the sensors are arranged in an arc shape across the mean wind (a near-circular arrangement for arbitrary wind direction). The distance between the source and the detection sensor can be estimated from formulas from published literatures in other studies (*4, 5*). The distance-spreading relationship is related to the atmospheric stability conditions, with wider spreading in unstable, slower wind conditions, and narrower spreading in stable and stronger wind conditions.

After searching for the source area using the puff backward trajectory computation, the source inversion system applies the dynamical Bayesian inference theory (*6, 7*) to "fine-tune" the release location and find the release characteristics. Let **α** be a time series of the dispersion parameter vector (the source location and strength), $\alpha \equiv (\alpha_1, \ldots, \alpha_t)$, and **β** be a time series of detected concentration data, $\beta \equiv (\beta_1, \ldots, \beta_t)$. The posterior, $\pi(\alpha)$, a conditional probability of system parameters with respect to the observational data, can be expressed as follows using the Bayesian rule:

$$\pi(\boldsymbol{\alpha}) = \frac{p(\boldsymbol{\beta}/\boldsymbol{\alpha})p(\boldsymbol{\alpha})}{p(\boldsymbol{\beta})} \propto p(\boldsymbol{\beta}/\boldsymbol{\alpha})p(\boldsymbol{\alpha}) \, , \tag{2}$$

where $p(\boldsymbol{\beta}/\boldsymbol{\alpha})$ is the likelihood (the conditional probability function of model output with respect to model parameters), $p(\boldsymbol{\alpha})$ is the prior distribution, and $p(\boldsymbol{\beta})$ is the marginal probability distribution of **β**. The computation of $p(\boldsymbol{\beta})$ is prohibitively expensive. Instead of trying to compute it directly, an alternative approach is to generate a collection of realizations from the posterior distribution and use these samples to conduct inference (*6, 7*). The likelihood function $p(\boldsymbol{\beta}/\boldsymbol{\alpha})$ accounts for the information of the forward dispersion model and detection sensor. It needs special treatment for the errors due to the sensor threshold limits and range limit. When the concentration is below the sensor detection threshold, the reading from the sensor is zero. When the concentration is exceeding the sensor saturation value, the instrument reading is set to the saturation level. Following the treatments of other investigators (*8–11*), the likelihood function $p(\boldsymbol{\beta}/\boldsymbol{\alpha})$ can be expressed as the following function:

$$p(\boldsymbol{\beta}/\boldsymbol{\alpha}) = \exp \left[-\sum_{ij} \frac{(\log M_{ij} - \log C_{ij})^2}{2n\sigma^2} \right], \tag{3}$$

where M_{ij} and C_{ij} are the observed concentration and forward model produced concentration, respectively, at location i and time j, n is the number of sensors in the detection network, and σ is the error parameter, which incorporates both the errors in the sensor detection and in the forward

model. Other forms of likelihood function can be used (*7, 10*). The function is designed to capture the error information from the observations and the forward dispersion model. The error estimate in Bayesian inference is a complex research topic; further research is required. In the current experiment, a value of $\sigma = 0.15$ is taken for the combined error from observations and the forward model. A larger value of σ will yield a broader final posterior distribution.

The posterior distribution of $\pi_t(\alpha_{1:t})$ is generated from the Markov stochastic sampling procedure, named the Metropolis-Hasting method (*7, 12*), and computed from equation 2. The specific Metropolis sampling procedure for our system can be described as follows: The sampling process begins with a source parameter, $\alpha_1 \equiv (X_1, R_1)$, where X_1 and R_1 are the source location vector and release strength at step 1. The X_1 starts at the previous backward trajectory obtained region, and R_1 starts at a reasonable guess of release rate. In the *i-th* iteration, a candidate state $\alpha^* \equiv (X_i, R_i)$ is sampled. The samples of unknown source parameters (X_i and R_i) are from a large set of possible X and R. These source parameters provide source location and release strength for the forward dispersion model to compute the concentration field at the sensor locations. The observed values and forward model prediction at the sensor locations are compared. Based on the comparison, the probability of source parameter X_i and R_i at *i-th* iteration is updated using the likelihood function and prior probability values of $\alpha \equiv (X_{i-1}, R_{i-1})$. If the comparison of the X_i and R_i are more favorable than the previous *(i-1)th* value, the sampled parameter is then retained for the next iteration step. If the X_i and R_i are less favorable parameters, they are not rejected automatically but determined by a random process with a uniform distribution. This ensures that the sampling process is not going to trap into a local optimal value (*7, 8*). During the iteration, a candidate source parameter (α^*) with probability $\rho(\alpha, \alpha^*)$ is computed in the follow equation:

$$\rho(\alpha, \alpha^*) = \min(\prod_{n=1}^{N} \frac{\pi_n(\alpha^*)}{\pi_n(\alpha)}, \ 1) , \tag{4}$$

where *n* is the number of sensors in the network and $\pi_n(\alpha^*)$ and $\pi_n(\alpha)$ are computed using equation 2. Typically, four Markov chains are used in the stochastic sampling process. The convergence is attained when the ratio of variance within chain to variance between chains is approaching unity (*6*). The final posterior distribution produces the most likely source parameters X and R. The final forward concentration prediction is the reconstructed concentration field.

3. Results

Before applying the inversion method to a complex urban environment, an experiment with a simple situation was performed. In this example, a release source reconstruction in an idealized suburban area was considered. The computation domain consisted of five buildings over a

gentle terrain (figure 1). The chemical detection sensors were arranged at ground surface in a circle enclosing the five buildings. The test was based on a simulated "truth" of an atmospheric release at the ground surface. The wind field was initialized with several logarithmic profiles. Applying the data of the terrain, the building height, and the initial wind profiles, the wind field was computed using the 3-DWF model. The wind field remained in a steady condition during the 20-min release period. A neutrally buoyant gas was released in an upwind area of the five buildings. The concentration field was simulated with a Lagrangian stochastic particle model (LSPM) (*13–15*), which was to be compared with the reconstructed field. The LSPM-type model is usually considered a more advanced and accurate approach for the air pollutant dispersion simulation (*13, 14*). Unlike the LGPM model, a large number of particles in LSPM are released and the turbulence effects are simulated with a random walk model. However, a much longer computation time (as much as 10× more time compared with the LGPM) is required for a LSPM model simulation. Details about the LSPM can be found in Wilson and Sawford (*13*) and Thomson (*14*).
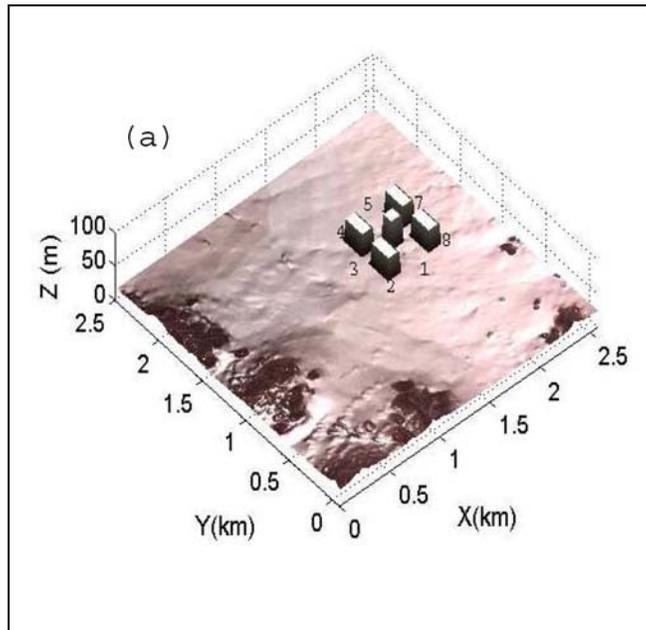
Figure 1. A 3-D diagram for the simulation domain.

Assume that in a real situation, the release source location and release strength are not known, only the concentration time series sampled (figure 2) from 6 out of the 8 sensors (in this simulated case). The wind field condition is monitored continuously. From the inspection of the time series signal (figure 2) and the wind field (figure 3), the release is continuous in a rather steady wind condition since the concentration signals reached the constant values for each sensor after about 100 s. The inverse system uses the information from the detection sensors and

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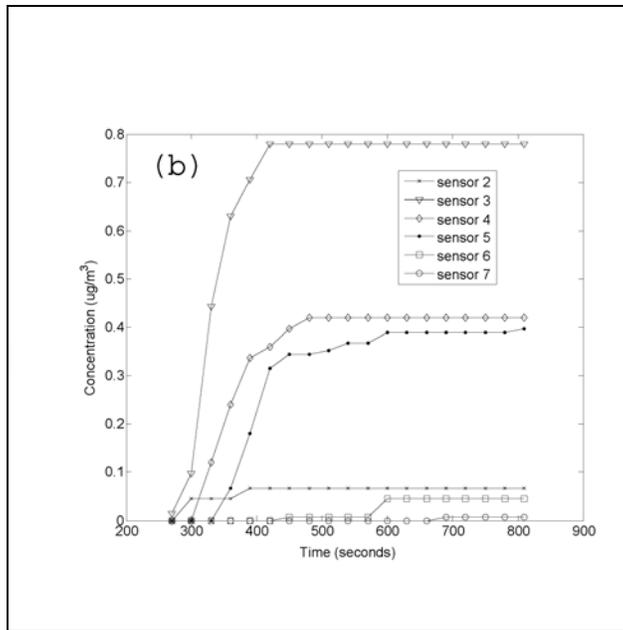
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sensors; sensors 1 and 8 have blank readings.
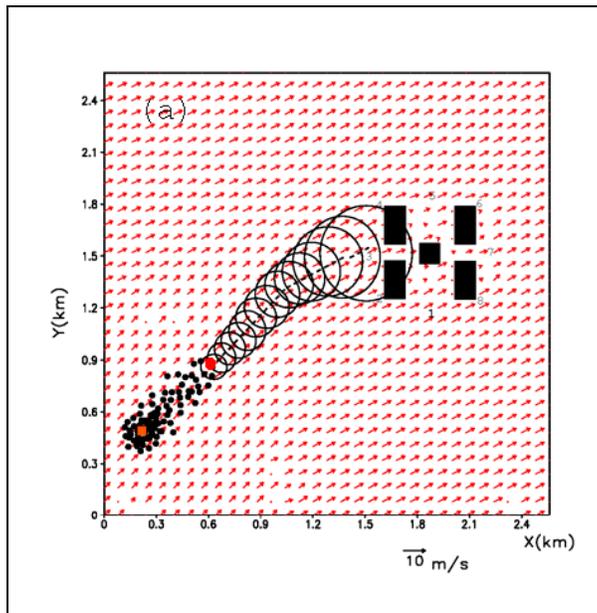
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4 m. The dashed line denotes the puff
backward trajectory, and the puff spreading
parameter is represented by circle radius.
The red dot is the starting point of a Markov
chain, and the red square is the release
location by the inversion method.

the wind field to reconstruct the source location and the release strength. The first step is to do a backward trajectory computation, starting at the sensor location with the maximum reading. This sensor location is considered as an approximated plume centroid location. The starting plume parameter, σ_h, is approximated from the line which is perpendicular to the wind at the sensor location. The σ_z parameter is taken as $0.75\sigma_h$ to start the backward trajectory computation for a neutral atmospheric stability condition. The plume source is traced back using the backward trajectory shown in figure 3, where the radiuses of the circles represent the σ_h values of the puff. The σ_h and σ_z values are computed using the formula from previous studies (5, 6). The puff centroid backward trajectory is computed by solving equation 1 using a second-order Runge-Kutta method. Since the purpose of the backward trajectory step is to reduce the computation in the entire source inversion system by tracing back to the approximated source location, the trajectory computation is stopped at the location with the $\sigma_h \sim 0.1$ km. At this time, the Markov chain Stochastic sampling process takes over to find the maximum likelihood estimate of release location and characteristics.

Four Markov chains started at the area where the puff backward trajectory was traced. The Markov chains sampled source locations and release strength, following the rules described in the Metropolis-Hasting method (7, 12). For clarity, figure 3 only shows the sampling locations from one Markov chain, where the starting point is marked by a red circle. The converging point is denoted by a small red square. The sampling starting point is proven to be near the release point with the help of backward trajectory. If the reconstruction system was not preceded with a backward trajectory computation, the Markov chain stochastic sampling would take much longer. The sampling starting location could have started at a location far away from the release location, taking much more iterations to converge to the release point. The system has been tested without using the backward trajectory procedure starting at random locations in the computational domain. Retrieving the release location would take as much as 4 hr of CPU time (~3× the computation time with default inversion system) on a 3-GH workstation to converge to the release point. At the same stochastic sampling process, the release strength was statistically retrieved in the Bayesian procedure. The sampling started at the release strength of 1 g/s, carried out with the 0.1 increment of release strength for a sampling iteration. The resulting release strength sampling is shown in a probability distribution in figure 4. It indicated that the largest posterior probability is approximately corresponding to the "true" release strength in the base simulation. The maximum likelihood estimate of the release strength is slightly greater than "true" release strength of 3 g/s. Using the reconstructed release location and release strength, a concentration field is computed as shown in figure 5. The comparison with the base simulation (figure 6) indicated that the release was satisfactory in this simple situation.
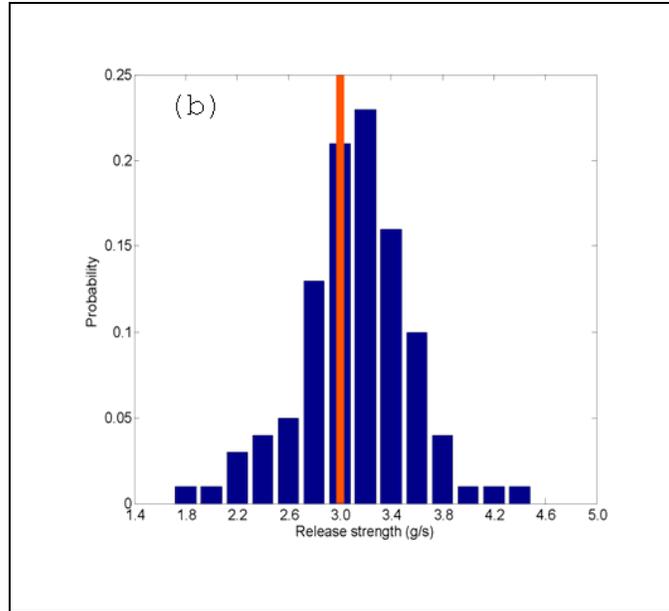
Figure 4. The sampling frequency for the release strength.
The red line is the "true" release strength.
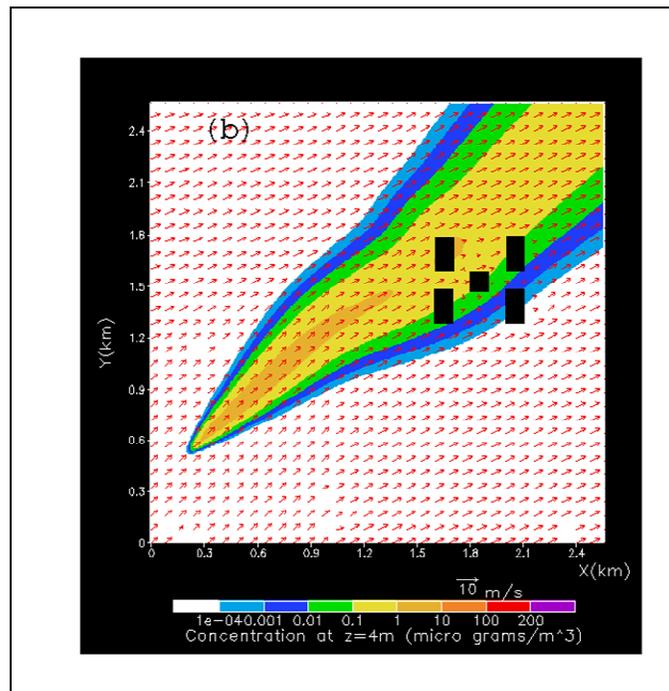
Figure 5. The reconstructed plume using the inversion method.
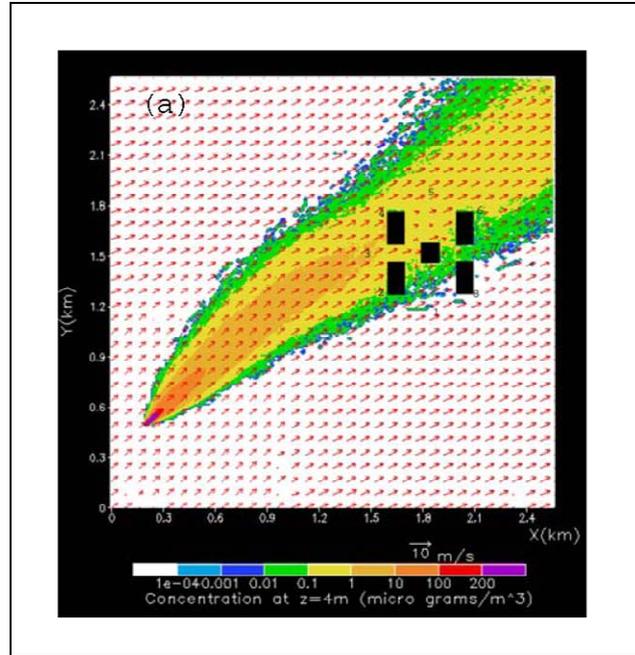
Figure 6. The simulated "truth" plume using the LSPM in
3-DWF computed wind field.

4. Conclusions

A source inversion method for reconstruction of the surface atmospheric release source location and strength has been developed in this research. The inversion system consists of a backward puff trajectory computation and a Bayesian inference process via stochastic sampling. The backward puff trajectory computation is used to trace back the approximated area of release location. The approximated area from the backward trajectory serves as a starting point for a Bayesian inference process. The Bayesian inference process is applied to search the release strength and the release location. A preliminary test with an idealized continuous, point source release case indicated that the method gives satisfactory inversion results in terms of the release location and strength. This integrated methodology combined backward trajectory and Bayesian inference reduces about 66% of the computation time compared with the method using the Bayesian inference only in a test case. Obviously, this is a preliminary exploration of the inversion method for a very simple situation. For real complex urban conditions, the following difficult issues need to be resolved: (1) the complex turbulence characteristic in the urban environment, (2) the backward trajectory computation in an urban environment, (3) the computation speed of the inversion system, and (4) the forward modeling of the plum or puff in different atmospheric stability conditions.

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