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STOCHASTIC EVENT RECONSTRUCTION OF ATMOSPHERIC CONTAMINANT DISPERSION

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1. INTRODUCTION

Event reconstruction of chemical or biological (CB) agent dispersion into the atmosphere is an important topic in homeland security and environmental monitoring, and it constitutes an inverse problem. In event reconstruction, also referred to as source characterization or source inversion in different studies, the major goal is to characterize the source of a contaminant or CB agent dispersion event in terms of release location and amount by using information from a sensor network, which can be available in the form of time-averaged concentration and wind measurements from scattered locations. Early detection of the CB agents with quick and accurate reconstruction of the dispersion events is critical in organizing an emergency response. Once the dispersion event is characterized, forward projections can be performed to analyze the extent of exposure to the contamination.

Event reconstruction of atmospheric contaminant dispersion has received a growing interest in recent years. Several studies have appeared in solving the problem with different methods. For instance, Keats et al. (2007) presented a Bayesian inference method for determining the source of a dispersion event within complex urban environments. A source-receptor relationship was incorporated into the likelihood function by solving an adjoint equation for the scalar concentration, which was found to be efficient in decreasing the overall calculation time.

Thomson et al. (2007) applied an inverse problem approach to locating a known gas source from measurements of gas concentration and wind data. A search algorithm with simulated annealing method was employed to find the source location and its strength. The simulated annealing approach helps prevent the search algorithm to converge onto a local minimum that might surround the global minimum.

Allen and Haupt (2007) developed a source characterization method in which a forward dispersion model is coupled with a backward receptor model using a genetic algorithm. A second-order closure integrated puff model was used in the source characterization. The method was validated with both synthetic and experimental field data. Allen et al. [4] extended this method by considering the wind direction as an unknown parameter. Instead of the puff model, a simple Gaussian plume model was considered in their study.

Johannesson et al. (2004) presented dynamic Bayesian models using Monte Carlo methods for target tracking and atmospheric dispersion event reconstruction problems. Both the well established Markov chain Monte Carlo (MCMC) method and the sequential Monte Carlo method for dynamic problems are discussed in detail in their study.

Chow et al. (2006) and Neumann et al. (2006) extended the Bayesian event reconstruction method of Johanneson et al. (2004) for neighborhood scale atmospheric dispersion events. Both computationally intensive building resolving computational fluid dynamics models, and computationally less intensive empirically based Gaussian puff models were adopted in these studies, respectively. The results have shown that the Bayesian methodology is efficient in delivering probabilistic answers to the event reconstruction problem.

Depending on the complexity of the forward model, the Bayesian approach to inverse problems can be computationally intensive in terms of the overall execution time. In the event reconstruction problem, the dispersion models are typically executed for many times within the MCMC framework in order to sample from the posterior distribution. It should be noted that MCMC chains converge onto the source location quickly, but chains are actually executed longer in order to deliver results with uncertainty, which is important in emergency response operations. With simple fast-response dispersion models, the overall execution time for MCMC chains is less of a problem, but with high-fidelity models the issue can be a limiting factor in emergency response situations. To address this issue, Marzouk et al. (2007) reformulated the Bayesian approach to inverse problems by adopting polynomial chaos expansions to represent random variables. In their study, a transient diffusion problem was considered. The results have shown that significant gains in computational time can be obtained by adopting the new scheme over direct sampling.

In what follows, a stochastic event reconstruction method is presented, extending the Bayesian inference framework described in Johannesson et al. (2004) and Chow et al. (2006). Particularly, a probability model is proposed to take into account

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both zero and non-zero concentration observations that can be available from a sensor network. The parameters in the probability model are calculated from prior distributions, resulting in a method free from tunable parameters. Simple fast-running Gaussian plume dispersion models are adopted as the forward model in the Bayesian inference method. The event reconstruction method is validated using data from a tracer dispersion experiment (Erik and Lyck, 2002).

2. BAYESIAN FORMULATION

The forward modeling problem can be defined as predicting the response of a system, using a physical theory (forward model) and system parameters. In the inverse modeling problem, an inference is made on the values of the system parameters based on observations on the system response (Tarantola, 2005). Loosely speaking, inverse problems can be formulated as follows:

$$\mathbf{m} \approx F^{-1}(\mathbf{d}), \tag{1}$$

where **d** is a vector of observations, **m** is a vector of model parameters, and the operator *F* is the forward model that governs the system response. Inverse problems can be ill-conditioned, because small changes in **d** can lead to large changes in **m**. Depending on the nature of inverse problems; both deterministic and probabilistic approaches have been developed for solving them. Probabilistic approaches can be formulated within the context of Bayesian inference, which is pursued in the present study.

The present event reconstruction problem requires estimating the model parameters (**m**) (e.g. release location, amount of material released, wind direction etc.) given the observed concentrations (**d**) from a sensor network.

Bayes' theorem defines the posterior probability of a set of model parameters (**m**) given the observations (**d**) as follows (Gilks et al., 1996; Carlin et al., 1996):

$$p(\mathbf{m} \mid \mathbf{d}) = \frac{L(\mathbf{d} \mid \mathbf{m})\, p(\mathbf{m})}{p(\mathbf{d})}, \tag{2}$$

where $p(\mathbf{m}|\mathbf{d})$ is the *posterior probability density*, $L(\mathbf{d}|\mathbf{m})$ is the *likelihood function*, $p(\mathbf{m})$ is the *prior probability density*, and $p(\mathbf{d})$ is the *marginal probability density*. The posterior probability density given in Eq. (2) defines the conditional probability density of forward model parameters (**m**), given the observed data (**d**), Calculation of $p(\mathbf{m}|\mathbf{d})$ is central in Bayesian inference, and it can also be viewed as a solution to an inverse problem.

Direct computation of the posterior density, using Bayes' theorem, necessitates the computation of the marginal probability density $p(\mathbf{d})$, given in Eq. (2), which can be computationally intensive to the point of being impractical for most applications. A practical approach to estimate the posterior probability density is to perform MCMC sampling by noting the following (Metropolis et al., 1953; Gilks et al., 1996; Carlin et al., 1996)

$$p(\mathbf{m} \mid \mathbf{d}) \propto L(\mathbf{d} \mid \mathbf{m})\, p(\mathbf{m})\,. \tag{3}$$

Within this framework, the observed data (**d**) enters the formulation only through the ratio of likelihood function.

Specification of the likelihood function deserves attention, because it models how the observations are acquired. For instance, the sensor network cannot quantify the concentration of tracers below its threshold specification for detection, and registers a zero concentration value. Hence, a likelihood function is needed that accounts for zero sensor readings when in fact the actual concentration is non-zero.

Let **m** be the model, C_m the predicted concentration, ξ the concentration measured by an ideal sensor, and *d* is the concentration observed by an actual sensor. It is assumed that the observations *d* are related to ξ as follows:

$$d = \begin{cases} 0 & \text{with probability } e^{-\alpha C_m}, \\ \xi & \text{with probability } 1 - e^{-\alpha C_m}, \end{cases} \tag{4}$$

and ξ, given the model, has a lognormal distribution with density

$$p(\xi \mid \mathbf{m}) = \frac{1}{\sqrt{2\pi}\sigma\xi} \exp\left(-\frac{(\log\xi - \log C_m)^2}{2\sigma^2} \right). \tag{5}$$

In Eq. (4), it is assumed that the probability of not detecting a plume can be calculated based on the predicted concentration C_m, and at the threshold concentration C_{th}, the plume is detected with probability ½, from which α can be computed as

$$1 - \exp(-\alpha C_{th}) = \frac{1}{2} \;\rightarrow\; \alpha = \frac{1}{C_{th}} \log 2\,. \tag{6}$$

Then, the likelihood function can be calculated as follows:

$$\begin{aligned} L(d \mid \mathbf{m}) &= \int_0^\infty p(d, \xi \mid \mathbf{m}) d\xi \\ &= \mathrm{I}[d = 0] \int_0^\infty \exp(-\alpha C_m) p(\xi \mid \mathbf{m}) d\xi + \\ &+ \mathrm{I}[d > 0] \int_0^\infty [1 - \exp(-\alpha C_m)] p(\xi \mid \mathbf{m}) \delta_d(\xi) d\xi, \end{aligned} \tag{7}$$

where δ_d is the Dirac delta-function. Therefore the likelihood function can be written as:

$$\begin{aligned} L(d \mid \mathbf{m}) &= \mathrm{I}[d = 0] \cdot \exp(-\alpha C_m) + \\ &+ \mathrm{I}[d > 0] \cdot \frac{[1 - \exp(-\alpha C_m)]}{\sqrt{2\pi}\sigma d} \cdot \\ &\cdot \exp\left(-\frac{(\log d - \log C_m)^2}{2\sigma^2} \right). \end{aligned} \tag{8}$$

In emergency response situations, the overall run-time for delivering answers is an important factor. Hence, fast running Gaussian plume dispersion models are adopted as the *forward model* to compute C_m. A Gaussian plume dispersion model for uniform steady wind conditions can be written as follows (Panofsky and Dutton, 1984):

$$C_m(x,y,z) = \frac{Q}{2\pi U \sigma_y \sigma_z} \cdot \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \cdot \left[\exp\left(-\frac{(z-H_r)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H_r)^2}{2\sigma_z^2}\right)\right] \quad (9)$$

where C_m is the concentration at a particular location, Q is the release rate, U is the mean wind speed, H_r is the height of the release, x is the distance along the wind, y is the distance along the horizontal crosswind direction, and z is the distance along the vertical axis. Note that the release location is the origin for x, y and z directions. σ_y and σ_z are called the standard deviation in the horizontal crosswind and vertical directions, respectively. These two parameters are also known as the Gaussian plume dispersion parameters, and they are defined empirically for different stability conditions. For Pasquill C type stability, Briggs formulas for urban conditions parameterize the standard deviations as follows (Panofsky and Dutton, 1984):

$$\sigma_y = 0.22 \cdot x \cdot (1 + 0.0004 \cdot x)^{-0.5}, \qquad \sigma_z = 0.20 \cdot x. \quad (10)$$

Several formulas have been proposed for the standard deviations, and their particular forms remain to be problem specific. Results typically benefit from adjusting the empirical parameters. In the present study, some of the empirical constants that appear in the above formulas are treated as stochastic parameters within the Bayesian framework as shown below:

$$\sigma_y = C_1 \cdot x \cdot (1 + 0.0004 \cdot x)^{-0.5}, \qquad \sigma_z = C_2 \cdot x, \quad (11)$$

where C_1 and C_2 are stochastic parameters that replaces the empirical parameters 0.22 and 0.20 in Eq. (10), respectively. This approach allows one to calibrate the deficiencies in the forward dispersion model to certain extents, and helps improve the event reconstruction results significantly. Furthermore, in the posterior distribution, these parameters converge onto values that give better agreement with the observed data, which can be used in performing forward projections for the dispersion event under consideration.

The prior probability density term $p(\mathbf{m})$ in Eq. (3) represents prior knowledge about the model parameters (**m**) before observing the data (**d**), which can be expressed by assigning probabilities to model parameters (**m**) based on bounds on certain physical properties or expert opinions. For instance, data regarding the probabilities of possible wind directions acting on a city might be available from previous meteorological studies. Defining a prior probability is subjective and depends on the problem at hand. In the event reconstruction problem, since the release can originate from any location, one can assign a uniform prior probability to release location, and one may also assume that low release rates might be more likely than high release rates. Hence, the following can be written

$$p(\mathbf{m}) = p(\mathbf{r}) \cdot p(Q) \propto 1 \cdot \frac{Q_{\min}}{Q}, \quad (12)$$

where **r** is the release location and Q is the release rate, and $Q_{\min}$ is a user defined minimum emission rate that is of importance for a given problem. It should be emphasized that the above form is problem specific, and it depends on the available prior information about a specific event.

Various algorithms exist for MCMC sampling. In the present study, Metropolis algorithm is adopted to simulate samples from the posterior (Metropolis et al. 1953). The reader is referred to Gilks et al. (1996) and Carlin and Louis (1996) for a detailed explanation of the algorithm. In the Metropolis algorithm, a candidate state ($\mathbf{m}^*$) is sampled from a proposal distribution at each iteration, and the candidate state is accepted with probability

$$\rho(\mathbf{m},\mathbf{m}^*) = \min\left(\prod_{n=1}^{N} \frac{\pi_n(\mathbf{m}^*)}{\pi_n(\mathbf{m})}, 1\right), \quad (13)$$

where N is the total number of sensors in the network and **m** is the current state. When the MCMC algorithm has converged, it is expected that the proposal distribution draw samples from the target distribution, which is defined as

$$\pi_n(\mathbf{m}) = L(\mathbf{d} \mid \mathbf{m}) \cdot p(\mathbf{m}). \quad (14)$$

The above equation is computed using Eqs. (8) and (12). In Eq (8), the variance of the distribution (σ^2) is not specified, but it is calculated in the course of MCMC iterations from an inverse gamma prior distribution.

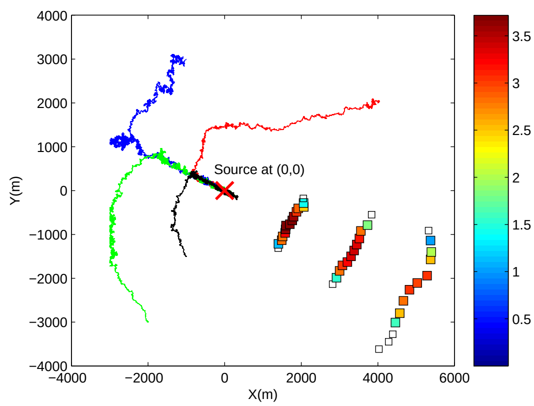

Figure 1: Traces of four independent Markov chains converging onto the contaminant release location. Square markers denote sampler/sensor locations colored with measured concentration levels in ng/m^3. Logarithmic (base 10) values are shown. Clear markers indicate sensors that registered zero concentration values.

3. RESULTS & DISCUSSION

Environmental sensor networks have been deployed in various cities, and specifics of these networks and actual data from the sensor network are not publicly available. Hence, direct testing of event reconstruction methods is not feasible. However, tracer field experiments designed for atmospheric dispersion and air pollution studies can be utilized in evaluating the performance of event reconstruction models. A series of tracer experiments were performed in the Copenhagen area in 1978 and 1979. Concentrations of tracer sulphurhexafluoride (SF6) and meteorological conditions were measured and reported in Erik and Lyck (2002). For all the experiments, tracer was released from a tower with a height of 115 *m*. Samplers/sensors were placed 2-3 *m* above the ground level along three crosswind arcs that are positioned 2-6 *km* away from the tracer release point. The location of the samplers is shown in Fig. 1. The total sampling time for the concentration measurements was 1 hour. In the tracer data corresponding to the experiment performed on October 19, the detection limit was given as 9 ng/m^3, and any value below this limit was indicated as zero. This value is used to set the sensor threshold value (C_{th}) in Eq. (6) of the stochastic event reconstruction method. Out of 40 samplers, 7 samplers registered zero concentration values.

In the following example, the tracer dispersion experiment is reconstructed in terms of the following parameters

$$\mathbf{m} = (x, y, H, Q, \theta, U, C_1, C_2, \sigma^2), \quad (15)$$

where x and y are the spatial locations of the release, H is the release height, Q is the release rate, θ is the wind direction, U is the wind speed at the release height, C_1 and C_2 are the stochastic terms in the turbulent diffusion parameterization given in Eq. (11), and σ^2 is the variance term in Eq. (8).

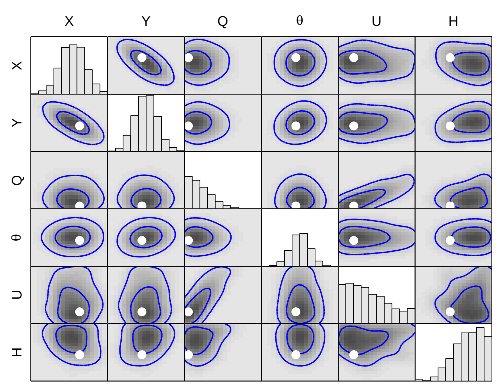

Figure 2: Multi-variate analysis of event reconstruction parameters. The white dot represents the true value from. The outer and inner contour lines indicate 90% and 50%, respectively.

Fig. 1 shows traces of four different Markov chains converging on the source location. The locations of the samplers are also indicated in this plot, and they are colored with the one hour averaged concentration measurements. Fig. 1 clearly shows that chains converge on the source location independent of the starting point.

In typical emergency response operations, finding the location of the release is one of the primary goals. Probabilistic answers instead of deterministic answers are preferred due to the nature of operations. Hence, posterior distributions need to be mapped in terms of probabilities. The high dimensionality in the stochastic inversion process requires a careful check using multi-variate analysis. For that purpose the results are analyzed on a so-called trellis plot as shown in Fig. 2. The plots on the diagonal are the marginal probability distributions of the forward model parameters. The off diagonal plots are the joint posterior distributions of the forward model parameters. 90% and 50% contour lines are also overlayed on the joint posterior distributions. The true answer from the field experiment is highlighted with white colored circles on each subplot.

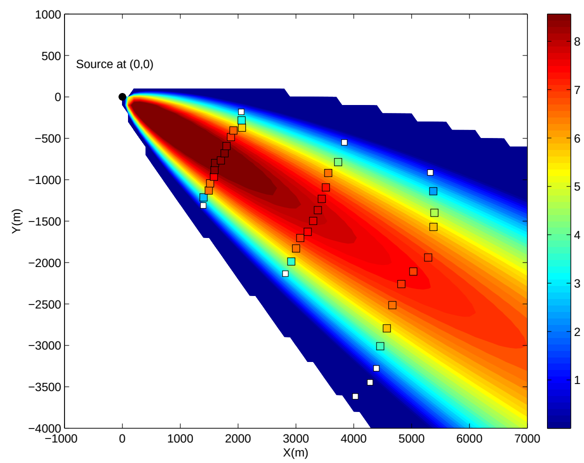

Figure 3: Probabilistic plume envelope for 95% confidence level. Concentration unit is ng/m3 and logarithmic (base 10) values are plotted. Clear markers indicate sensors that registered zero concentration values.

In atmospheric dispersion events, it is important that emergency responders are provided with results that incorporate uncertainty involved in the problem. The present Bayesian inference framework is convenient for addressing that need. Fig. 3 presents a probabilistic plume envelope with a confidence level of 95%. The plume envelope is generated by running a forward model for each posterior sample and storing the concentrations on a vector at desired locations. Then, the concentration value corresponding to the 95th percentile in the data is selected as the probabilistic plume envelope that gives a confidence level of 95%. As can be seen from Fig. 3, the plume envelopes all the samplers/sensors. Hence, in analyzing this plot, one can have 95% confidence in assuming that the actual concentration is what the plot indicates or below. Fig. 4 provides a check of this assumption. Concentration data from the probabilistic plume envelope is compared against the actual measurements from the samplers on a scatter plot. Clearly, about 95% of the data is overpredicted by the simulation that would allow safer decisions in case of harmful dispersion events.

Fig. 5 shows the histograms of the stochastic parameters given in Eq. (11). The constant empirical parameters given in Eq. (10) are also overlaid on this plot. As can be observed from this plot, the stochastic terms converged onto different values.

Use of Eq. (11) greatly improved the event reconstruction results. As shown in Fig. 6, the event reconstruction method adopting Eq. (10) in the Gaussian plume model is not successful, because the MCMC chain converges onto a zone that does not include the true source location. However, the event reconstruction method that adopts Eq. (11) is deemed successful, because the MCMC chain converges onto a zone that includes the true source location.

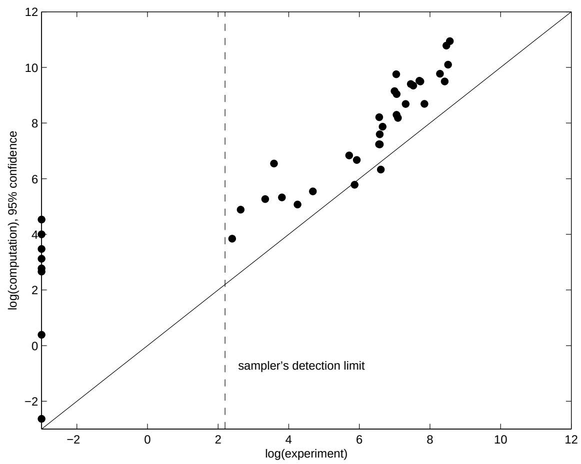

Figure 4: Scatter plot of probabilistic plume envelope (95% confidence level) vs. measurements.

4. CONCLUSIONS

A stochastic event reconstruction method for atmospheric contaminant dispersion is presented. The method is based on Bayesian inference with MCMC sampling. The Bayesian approach provides a convenient framework to propagate uncertainty to the final event reconstruction results. To address the fast-response operational needs, simple fast-running Gaussian plume dispersion models are adopted as the forward model in the inverse problem.

A probability model is suggested to take into account both zero and non-zero concentration measurements that can be available from a sensor network because of sensor's detection limit. Variance term in the likelihood function is considered as unknown, and it is calculated from an inverse gamma prior distribution, resulting in an event reconstruction method free from tunable parameters.

In practice, the release location and release rates are of great importance to the emergency responders. It is shown that the event reconstruction problem can be posed with many unknown parameters. In the event reconstruction of Copenhagen tracer experiment, up to 9 parameters are treated as unknowns. It is found that stochastic treatment of the empirical parameters of the Gaussian plume dispersion model, improves the event reconstruction results significantly. This approach allows the optimization of the dispersion model according to the observations. In the posterior distributions, stochastic parameters that appear in Eq. (11) converge on to values specific to the dispersion problem at hand, which can also be used in post-event dispersion projections.

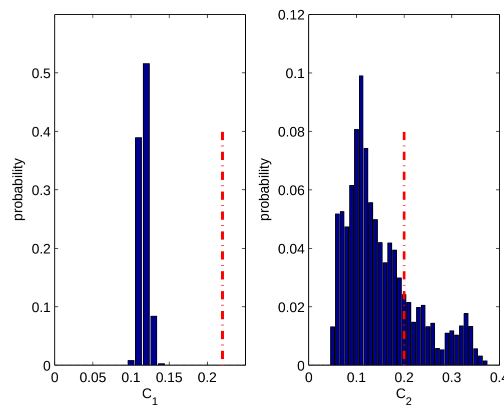

Figure 5: Histogram of stochastic parameters given in Eq. (11). The dashed lines locate the constant empirical values given in Eq. (10).

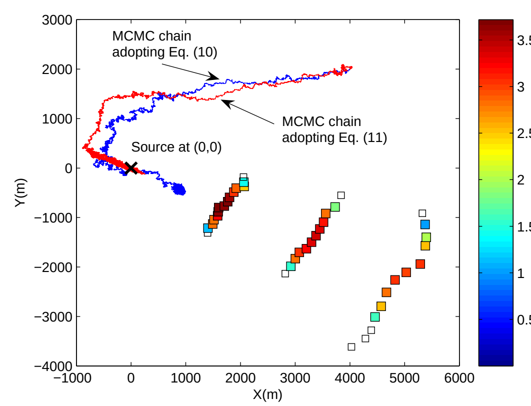

Figure 6: Comparison of the traces of two MCMC chains. The red and blue chains belong to event reconstruction methods that adopt Eq. (11) and Eq. (10) in the Gaussian plume model, respectively

The simulations have shown that the stochastic event reconstruction method is successful in capturing the true answers within the posterior distribution. Posterior distributions of the unknown parameters were also used to generate probabilistic plume envelopes with specified confidence levels.

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