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LOCATING THE SOURCE OF ATMOSPHERIC CONTAMINATION BASED ON DATA FROM THE KORI FIELD TRACER EXPERIMENT

Accidental releases of hazardous material into the atmosphere pose high risks to human health and the environment. Thus it would be valuable to develop an emergency reaction system which can recognize the probable location of the source based only on concentrations of the released substance as reported by a network of sensors. We apply a methodology combining Bayesian inference with Sequential Monte Carlo (SMC) methods to the problem of locating the source of an atmospheric contaminant. The input data for this algorithm are the concentrations of a given substance gathered continuously in time. We employ this algorithm to locating a contamination source using data from a field tracer experiment covering the Kori nuclear site and conducted in May 2001. We use the second-order Closure Integrated PUFF Model (SCIPUFF) of atmospheric dispersion as the forward model to predict concentrations at the sensors' locations. We demonstrate that the source of continuous contamination may be successfully located even in the very complicated, hilly terrain surrounding the Kori nuclear site.

Keywords: *sequential Monte Carlo methods, accidental releases into the atmosphere, emergency reaction system*

1. Introduction

Accidental releases of harmful material into the atmosphere pose a significant risk to human health and the environment. In the case of such sudden releases of chemical,

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radioactive or biological material, emergency responders need to determine the location of the source as soon as possible.. Such information is necessary to make rapid and effective decisions regarding people's safety, evacuation plans and the management of emergency services. In this context, it is important to develop an emergency system that is based on measurements of the concentration of a dangerous substance by a network of sensors aimed at estimating the most probable location of the source of atmospheric contamination.

Knowing the source of an emission and wind field, an appropriate atmospheric dispersion model can be employed to calculate the expected concentration of a pollutant at any downwind location. On the other hand, given the concentration of a pollutant and knowledge of the wind field and other atmospheric parameters, locating the source of pollution and its parameters is a difficult problem. This problem has no unique solution and can only be considered in probabilistic frameworks.

The goal is to create a model of atmospheric dispersion which accurately reproduces the real situation based only on sparse point-concentrated data. This requires specifying the parameters of the model. In the framework of Bayesian statistics, all the quantities included in a mathematical model are modeled as random variables with a joint probability distribution. This probability distribution describes our uncertainty regarding the real values of the parameters. Bayesian methods reformulate the problem into searching a solution based on the efficient sampling of an ensemble of simulations, guided by comparisons with the data.

The problem of locating a source of pollution has been studied in the literature using both deterministic and probabilistic approaches. In [14], an algorithm was implemented based on integrating the adjoint of a linear dispersion model backward in time, to solve an inverse problem. In [9, 10], dynamic Bayesian modeling and Markov chain Monte Carlo (MCMC) sampling approaches were introduced to locate the source of a contaminant based on synthetic data.

Locating a source in an urban environment was discussed in [11] and [3]. In [11], an adjoint representation of the source-receptor relationship was used. The authors used Bayesian inference in conjunction with MCMC sampling procedures. This approach was validated using data from simulations of a water channel and a field experiment (Joint Urban 2003) in Oklahoma City.

In [3], the method presented in [16] was applied to the reconstruction of the flow around an isolated building and the flow during IOP3 and IOP9 of the Joint Urban 2003 Oklahoma City experiment. In these experiments, the source was inferred to be located 70 m from the actual location of IOP3 (within a 400 m × 400 m domain). In the case of the IOP9 model, errors and other uncertainties limited the ability of the algorithm to pinpoint the location of the source. In this reconstruction, the FEM3MP model was applied to simulate atmospheric dispersion.

In [14], the authors applied the inversion algorithm presented in [16] to a continental-scale, accidental release of radioactive material from near Algeciras, Spain in

May 1998. The simulation of forward dispersion conducted in this study used the Lagrangian operational dispersion integrator (LODI) model [6]. The posterior distribution of the location of the source was a roughly bimodal distribution, with the modes located a few dozen kilometres north of Algeciras and less than 100 km downwind of the real location of the source.

In [1, 2] we tested a methodology combining Bayesian inference with MCMC methods adapted to the problem of real-time, data-driven search for a source of pollution based on synthetic experimental data. We demonstrated the advantage of algorithms that in various ways use prior probability distributions of the parameters describing the location of a source, based on available measurements, to update the marginal probability distributions of the parameters considered. The application of Sequential Monte Carlo (SMC) methods combined with Bayesian inference to the problem of locating the source of atmospheric contamination based on synthetic experimental data was presented in [20].

In this paper, we describe in detail the opportunity to combine MCMC and SMC with a Bayesian approach, in order to improve the accuracy of event reconstruction. To test the accuracy of the proposed algorithm, we use the SF_6 concentrations from the field tracer experiment conducted in May 2001 around the Kori nuclear site [17] as input data.

2. Specification of the domain and the dispersion model applied

From 2000 to 2002 six field tracer experiments were conducted at the Kori site in the east of Korea [8]. These experiments were carried out for the purpose of analyzing the site-specific characteristics of atmospheric dispersion and testing the FADAS real-time system of radiological dose assessment (Following Dose Assessment System) [7]. In this paper, we use data from the 3rd experiment carried out on 31st May 2001. The tracer gas SF_6 released from a meteorological tower (58 m high) with average rate 75.79 kg/h. The release started at 12:30 and lasted for 3.5 h. Sampling of the tracer took place every 10 min from 15:00 to 16:00. A total of 140 tracer gas samplers were placed on two lines along roads along radii of about 3 km and 12 km from the release point, respectively. During the experiment, meteorological data were also measured at several locations. The topography of the area, meteorological towers, sampling points and point of release are presented in Fig. 1.

During event reconstruction, in the forward model of atmospheric dispersion it is important to use information about the parameters characterizing the state of the atmosphere that can influence the transport of the dispersed substance. In the case of the Kori tracer experiment, one of the most important factors is the wind field. This experiment took place close to the south-east coast. During the daytime, the predomi-

nant wind blows from the south-east according to the effects of a land sea breeze. For this reason, the wind patterns are very complicated and coupled to a complex, hilly topography.

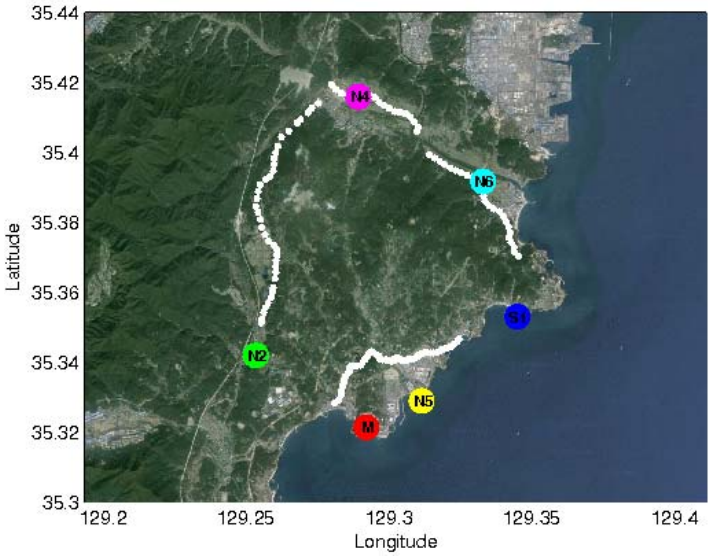

Fig. 1. Location of the point of release (*M*), sampling points (smaller dots) and meteorological towers (remaining dots) during the field tracer experiment conducted on 31st May 2001 around the Kori nuclear site

Another important factor is the choice of a model of atmospheric dispersion. This model is required to calculate the predicted concentrations that will be compared to the measured ones. The applied dispersion model cannot be very complicated, since computation time is crucial. Moreover, advanced dispersion models require the specification of numerous parameters, which leads to the parameter space becoming very complex. In many papers, e.g. [15, 16], the Gaussian plume dispersion model (e.g. [19]) is applied as a forward model. However, this model cannot take into account the changes in the wind field that must be taken into consideration.

For these reasons, we decided that the second-order Closure Integrated PUFF Model (SCIPUFF) is an appropriate dispersion model for the reconstruction presented in this paper. SCIPUFF is a model of atmospheric dispersion with a broad range of application. It uses a collection of Gaussian puffs to represent an arbitrary three--dimensional, time-dependent concentration field and incorporates an efficient scheme for splitting and merging puffs. The details of this model are described in [18].

We would like to underline that the only information used in the reconstruction procedure is the wind speed, wind direction and stability class recorded every 15 min by 5 meteorological towers at the height of 10 m from 12:30 to 16:00 (Fig. 2) and the

concentrations of the SF_6 gas registered every 10 min from 15:00 to 16:00 (i.e. 2.5 h after the start of the release). Based on these data, we try to infer the location of the contamination source (x, y) within a 15 km × 15 km domain and the release rate q. In consequence, the parameter space is $M \equiv \{x, y, z\}$, while the input data D are the concentrations at six time points.

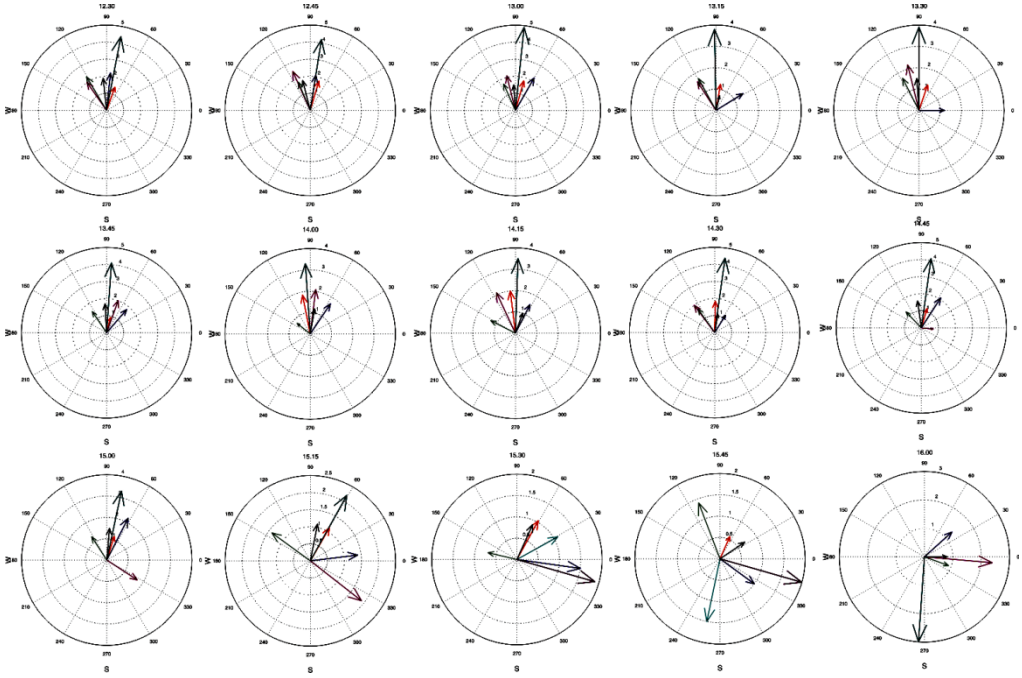

Fig. 2. Measurements of wind velocity during the field tracer experiment conducted on 31st May 2001 around the Kori nuclear site

3. Bayesian inference for the reconstruction problem

Bayes' theorem, as applied to a problem involving serious contamination, can be stated as follows:

$$P(M|D) \propto P(D|M)P(M) \tag{1}$$

In our problem, Bayes' theorem describes the conditional probability, $P(M|D)$, of the parameters of a particular source (model configuration M) given the concentra-

tions registered at sensor locations (D). This conditional probability, $P(M|D)$ is also known as the posterior distribution and is related to the probability of the data under a given model, $P(D|M)$, and of the possible models, $P(M)$, before the measurements made by the sensors are taken into account. The conditional probability of the data $P(D|M)$ is called the likelihood function, while $P(M)$ is the prior distribution. The likelihood of the data is computed by running a forward dispersion model with the given source parameters M and comparing the concentrations of the pollutant at the sensors as predicted by the model with those registered, D. The closer the predicted values are to the measured ones, the higher is the posterior likelihood of the parameters describing the source.

To estimate the unknown parameters of the source, M, the posterior distribution $P(M|D)$ must be sampled. $P(D|M)$ quantifies the likelihood of a set of measurements D given the parameters of the source M. The value of the conditional likelihood of the data is computed by running a forward dispersion model with the parameters M and comparing the concentrations predicted by the model with the actual data D, observed at the sensors using:

$$P(D|M) \equiv \sum_{i=1}^{NS} \left(\log\left(C_i^M\right) - \log\left(C_i^E\right) \right)^2 \tag{2}$$

The C_i^M are the concentrations predicted by the model at sensors i, C_i^E are the measurements made by sensor i, and NS is the number of sensors. Taking the logarithms of both the predicted and measured values prevents large concentrations from dominating in the computation of the likelihood. Both predictions and observations are set to the minimum detectable value when they fall below it, to ensure Eq. (2) can be evaluated. The same function was applied in [12, 14].

To obtain the posterior distribution of the parameters of the source, $P(M|D)$, based on a sampling procedure, we apply a hybrid SMC and MCMC approach using the Metropolis–Hastings algorithm. In this way, we completely replace the Bayesian formulation with a stochastic sampling technique to explore the parameter space of models and to obtain the probability distribution of the location of the source taking into account all the hitherto reported concentrations of the released substance.

4. The hybrid reconstruction procedure

Methods for simulating dynamic processes to obtain probability distributions for general dynamic models have been developed to overcome certain problems inherent

in classical MCMC methods. In many cases, classical MCMC implementations are unattractive. In particular, when we consider on-line data processing, standard samplers find it difficult to search the state space quickly enough [13]. In these situations, sequential Monte Carlo techniques are more efficient.

SMC is designed to sample from dynamic posterior distributions, in terms of both using the dynamic nature of the model and also reusing previous calculations. In [4], the authors presented the state of the art insequential Monte Carlo methods and introduced practical examples of using SMC. The SMC algorithm needs some set of samples to be initialized. One of the ideas is to use independent, parallel MCMC Metropolis–Hastings procedures and pass on the states of all the chains obtained as samples with associated weights to the SMC procedure (an outline of the algorithm is presented in Fig. 3). In the presented reconstruction, the SF_6 concentrations are reported by the sensors at six regularly-spaced time points. The proposed reconstruction algorithm starts to search for the location of the source (x, y) and release rate (q) just after the first set of measurements by the sensors (based on the data at time $t = 1$). Thus, a scanning algorithm is run on obtaining the first measurements. The parameter space scanned is $M \equiv \{x, y, q\}$. To reduce the size of the parameter space scanned and speed up the reconstruction (crucial in practical applications), we fix the height of the point of release to be 50 m (ca. 8 m below the actual height). Additionally, based on the wind pattern we have estimated that the release might have started at least 2 h before the first measurements. These assumptions of course influence the accuracy of the reconstruction, but are acceptable from a physical point of view.

Initially, we do not have any specific knowledge about the parameters describing the source, so we consider a 'flat' prior distribution $P^1(M) \equiv U(M)$, where $U(M)$ denotes the continuous uniform distribution over the whole space of parameters. Thus, for time $t = 1$, the first location of the Markov chain m_0^t is drawn from the prior distribution. The proposal is taken from $q\left(.\middle|m_i^t\right)$, thus it depends on the current state m_i^t. In the case of the reconstruction, to sample from $q\left(.\middle|m_i^t\right)$, we use a random walk procedure based on the Cauchy distribution, which allows larger increments in the parameters than the usually applied Gaussian distribution, resulting in the whole parameter space being scanned rapidly.

In standard applications, Markov chains move in one dimension per iteration. However, to optimize the time required to approach the target joint distribution of all the parameters, in the initial 80% of iterations the Markov chains simultaneously move in all directions in a single iteration. Then, to more clearly identify parameters that do not affect the likelihood function much, the chain randomly selects one dimension. The details are presented in Algorithm 1. The value α is the probability of accepting a new state $\breve{m}$. It is important to note that the condition $u < \alpha$ is likely to be

satisfied if the likelihood of the proposal is only slightly lower than the present likelihood. This gives a good chance of choosing a "slightly worse" state than the present one, because the probability of acceptance depends directly on the quality of the proposed state. Of course, if the state $\breve{m}$ is "better" than the previous one, the probability of acceptance equals 1.

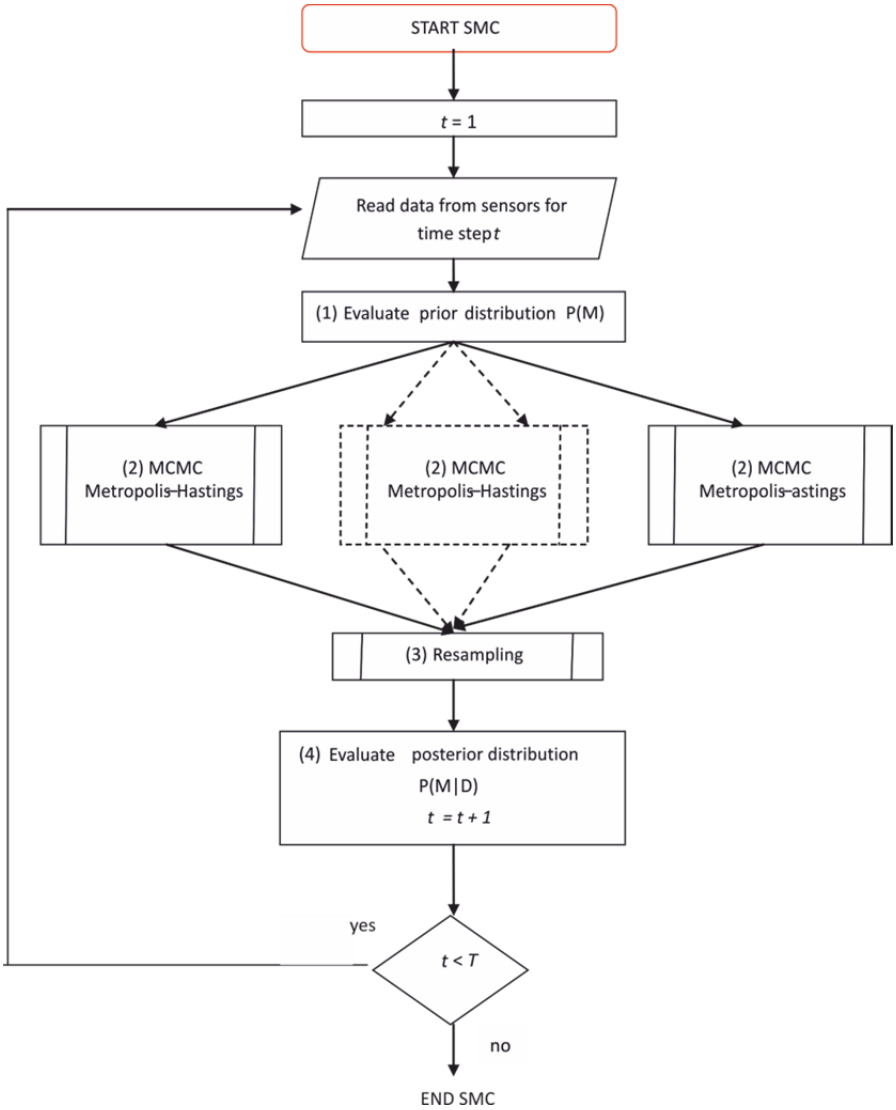

Fig. 3. A block diagram describing the Hybrid Reconstruction Procedure

Algorithm 1. MCMC Metropolis–Hastings

$m_1^t \sim P^t(M)$

Select initial position value from prior distribution →

for $i = 1$ to n do

propose a new state →

- $\breve{m} \sim q\left(.\middle| m_i^t\right)$

evaluate probability of acceptance →

- $\alpha = \min\left[1,\ \dfrac{P\left(\breve{m}\middle| d^t\right)}{P\left(m_i^t\middle| d^t\right)}\right]$

take a random number from uniform distribution →

- $u \sim U(0,1)$

if $u < \alpha$, then

accept a new state →

$$m_{i+1}^t \leftarrow \breve{m}$$

else

do not accept any new state →

$$m_{i+1}^t \leftarrow m_i^t$$

end if
and for

The basic idea of the SMC method is the resampling procedure [4, 10]. Resampling eliminates states that have small normalized weights. The probability of selecting a state from the set $m_0^t, m_1^t, ..., m_n^t$ depends on its quality. The main feature of this resampling is to focus on highly weighted states for which the likelihood function is the greatest and fill the output set of parameters with these states. The details are presented in Algorithm 2.

Algorithm 2. Resampling procedure

Take states from all *k* realizations of MCMC M–H →

Read $m_0^t, m_1^t, ..., m_n^t$

Calculate the state weights →

- $w_i \propto P\left(m_i^t \middle| d^t\right)$ for $i = 1, ..., n$

Normalize weights →

- $w_i \leftarrow \frac{w_i}{\sum_{j=1}^{n=k} w_j}$ for $i = 1, ..., n$

Draw with replacement from the discrete set of states →

for i = 1 to N do

Take a new state $\hat{m}_i^t$ according to the discrete distribution over the set $m_0^t, ..., m_{nk}^t$ with the probability

- $P\left(m_l^t\right) = w_i$ for $l = 1, ..., nk$

Assign new weights →

- $\hat{w}_i = \frac{1}{N}$

end for

4.1. Posterior distribution

Based on the resampled set of accepted samples, the empirical posterior probability distribution is computed as:

$$P\left(M \middle| D\right) \equiv \hat{\pi}^t\left(m \middle| d^t\right) = \frac{1}{N}\sum_{i=1}^{N} \delta\left(\hat{m}_i^t - m\right) \tag{3}$$

where $\hat{\pi}^t\left(m \middle| d^t\right)$ represents the empirical conditional probability of a particular model *m* given the concentrations recorded during the time interval *t*. The sum is taken over

the sample set of length N containing all the sampled values $\hat{m}_i^t$. Thus $\delta\left(\hat{m}_i^t - m\right) = 1$ when $\hat{m}_i^t = m$, and 0 otherwise. If many sampled states correspond to the same location, the estimate of $P\left(M \middle| D\right)$ is relatively large (such parameters describing the source are deemed to be relatively likely).

4.2. Prior distribution

The method chosen to define the prior distribution $P^t(M)$ is crucial in the SMC procedure. In the first time step, we do not have any specific knowledge about the parameters, so we choose a "flat" prior $P^1\left(M\right) \equiv\sim U\left(M\right)$, where $U(M)$ denotes the continuous uniform distribution over the whole parameter space [1]. However, applying this "flat" prior in each time step of the reconstruction would not be an efficient approach. In [1], we investigated various versions of MCMC algorithms that use (or do not use) probability distributions based on the information from previous measurements as the prior distribution. We showed that the scanning algorithm is definitely more effective when it makes use of past realizations and updates the marginal probability distributions based on new measurements of concentration levels. Consequently, at time t, $t > 1$, the prior is calculated based on sampled states taken from the resampling procedure as follows:

$$P^t\left(M\right) \equiv U\left(\hat{m}_1^{t-1}, \hat{m}_2^{t-1}, ..., \hat{m}_N^{t-1}\right) \tag{4}$$

where U denotes the discrete uniform distribution over all the sampled states $\hat{m}_1^{t-1}$. One major advantage of this procedure is that there no need exists to explicitly estimate the state distribution. This approach also gives us the possibility of drawing various initial states from various chains created using MCMC procedures.

5. Results

The task of locating the source of atmospheric contamination based on sensor data from the 2001 Kori field tracer experiment is quite challenging. The main problem is the site of the experiment. The Kori site is located at the southern end of a peninsula and is surrounded by the sea on three sides. In such terrain, the wind field configuration is very complicated. As presented in Fig. 2, the wind direction recorded by the meteorological towers changed significantly over the course of the experiment, e.g. at station N6 even by 180° and by more than 90° at other towers. The 140 automatic gas

samplers were located along roads. Also, neighbouring sensors reported highly varying concentrations, e.g. one of two sensors located very close to each other returned a zero concentration, while simultaneously the other recorded a high concentration. Thus for the reconstruction we selected the 24 most stable sensors with non-zero records. In the calculations, we used 10 Markov chains with 10 000 iterations in each time step. This number was based on numerical experiments as being sufficient to reach convergence for each sample set of model parameters M. Statistical convergence was monitored by computing between-chain variance and within-chain variance, see e.g. [5, 2]. The burn-in time, the number of samples required to reach a point where the Markov chain is sampling from the target distribution, was fixed at 2000 iterations (the light, highly dispersed points in the top left of Fig. 4). Starting from the second-time step, a state drawn from the *a posteriori* distributions obtained in the previous time step was selected as the initial position of the Markov chain.

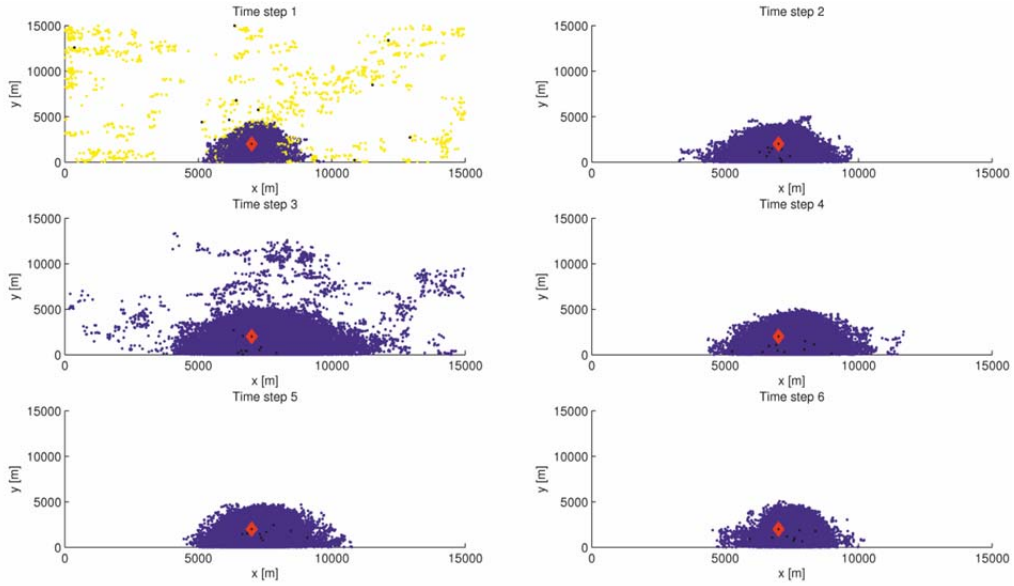

Fig. 4. The traces of 10 Markov chains in the location space (x, y) for all 6 time steps. The triangle marks the actual location of the source

Figure 4 presents traces of the Markov chains in the source coordinate space (x, y) at successive time steps. One can see that at the beginning, the sampled states are dispersed over the whole domain. Then, in each subsequent time step the calculations are updated using the posterior distributions and newly collected sensor data. This results in concentrating the accepted states around one point, the actual location of the source as marked by the diamond.

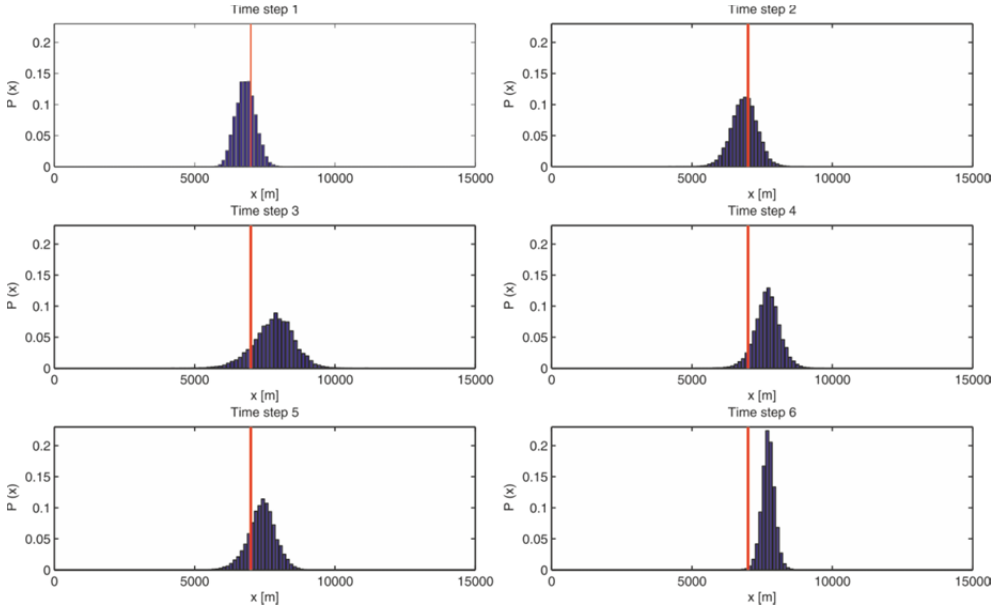

Fig. 5. The posterior distribution of the *x* coordinate of the source's location in successive time steps. The vertical line represents the target value of *x*

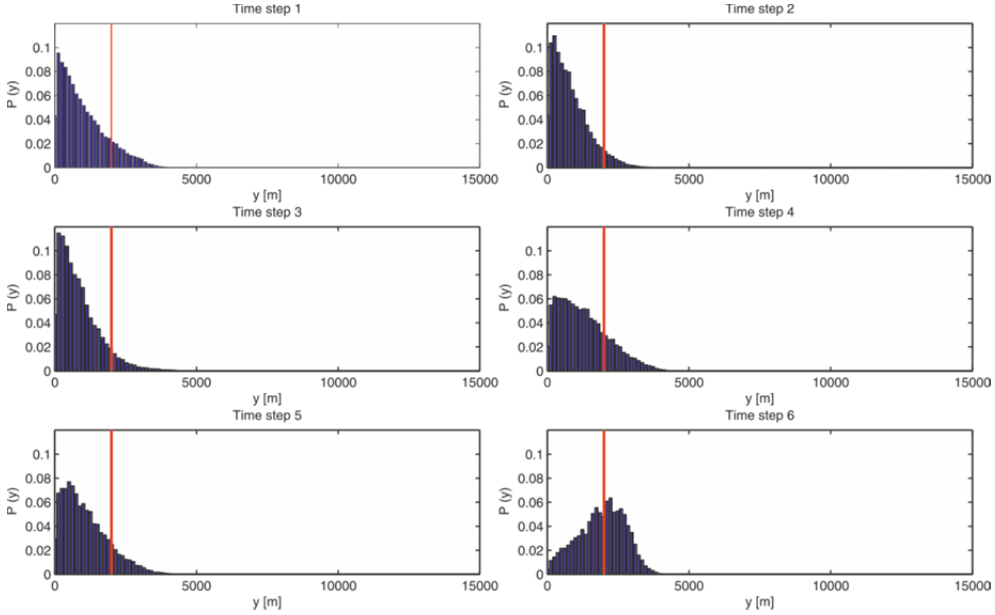

Fig. 6. The posterior distribution of the *y* coordinate of the source's location in successive time steps. The vertical line represents the target value of *y*

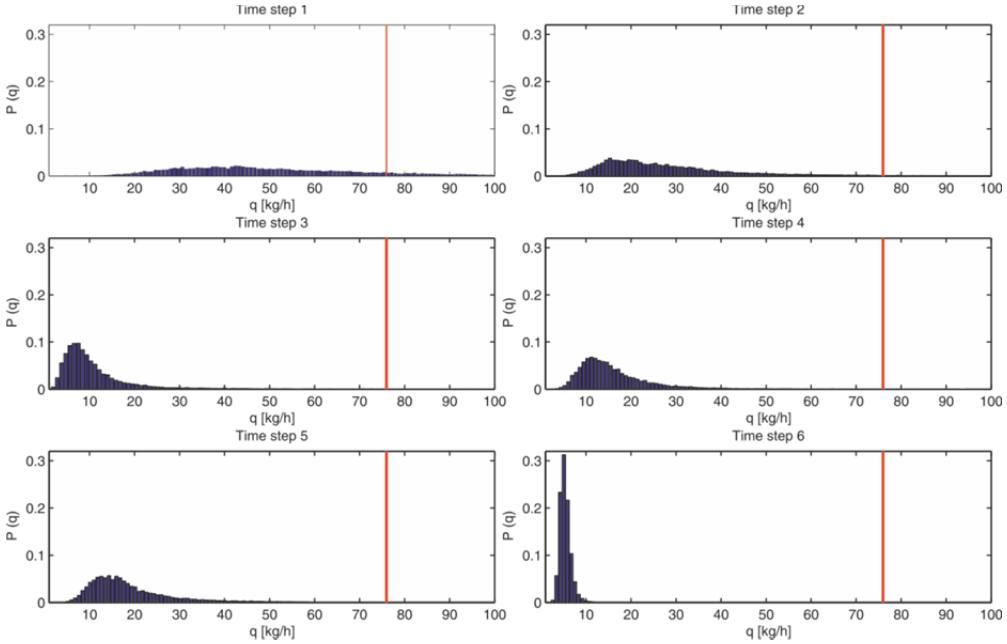

Fig. 7. The posterior distribution of the release rate q in successive time steps. The vertical line represents the target value of q

The *posterior* distributions of the parameters are presented in Figs. 5–7. Figure 5 shows that the distribution of the x coordinate starts to concentrate around the target value, $x = 7000$, early on in the procedure as indicated by the mode of the marginal distribution of x, $P(x = 6987 \pm 124) = 0.14$. In subsequent time steps, the peak of the distribution moves somewhat to the right of the target value and in the 6th time step the largest probability mass is $P(x = 7748 \pm 124) = 0.22$. However, at the same time, the estimate of the y coordinate improves. Initial estimation of the y coordinate does not agree with the target value. However, the final update of the *posterior distribution* using the concentrations recorded in the last time interval (6th time step) lead to the mode of the distribution of y being close to the target $y = 2000$), $P(y = 2293 \pm 124) = 0.06$. Comparing Figs. 5 and 6, one can observe that accurate estimation of the y coordinate takes place at the expense of precise estimation of the x coordinate. Figure 7 shows that estimation of the release rate via the reconstruction was highly inaccurate. The reason for this might lie in the facts that the complex terrain topography was only indirectly included in the model via the roughness coefficient and the release height was fixed in the forward dispersion model to be below its actual height.

3. Summary

We have presented a procedure to locate a source of atmospheric contamination based on a set of downwind concentrations. The dynamic data-driven method of event reconstruction developed combines Bayesian inference with Sequential Monte Carlo techniques and produces posterior probability distributions of the parameters describing the unidentified source. This approach successfully provides a solution to the inverse problem considered, i.e. the algorithm found the most probable location of the source based on measurements of the downwind concentration of pollutants and knowledge of the wind field.

The algorithm was tested with the use of the data from a field tracer experiment conducted on 31st May 2001 around the Kori nuclear site. We demonstrated that the location of a source of continuous contamination is successfully inferred even in the very complicated hilly terrain surrounding the Kori nuclear power plant. The coordinates of the source of contamination inferred to be the most probable by the reconstruction algorithm were close to the actual location of the source.

Acknowledgements

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