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ESTIMATION OF ATMOSPHERIC EMISSIONS BY AN ADAPTIVE MONTE CARLO MARKOV CHAIN METHOD

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Abstract. *The release of toxic gases into the atmosphere is a subject of great environmental concern. Such releases might occur in several ways, including in regular industrial activities and accidents. The proper identification of the origin and the quantity of released harmful materials is essential particularly in emergencies to avoid or reduce possible damages. To address such a relevant inverse problem, this work proposes a combination of accurate numerical techniques to model the dispersion in the atmosphere and to estimate emission sources from atmospheric releases. Considering a Bayesian inference framework, we propose the use of an adaptive Metropolis in Gibbs algorithm to estimate the sources and the so-called precision of the concentration measurements. The predicted concentrations necessary to solve this inverse problem are obtained from the numerical solution of an advection-diffusion partial differential equation given by a stabilized finite element method. The performance of the proposed algorithm is evaluated against experimental datasets.*

Keywords: *Source Identification, Bayesian inference, Adaptive MCMC, Air pollution.*

1. INTRODUCTION

The characterization of source parameters by data assimilation of measured concentration may require a large number of sensors, which can be an impractical task, especially during accidents or intentional releases. Thus, one of the main alternatives to identify pollutant sources and the amount of released materials is by inverse modeling.

The estimation of unknown source parameters using inverse problems techniques involves several steps. The first one is the proper characterization of a dispersion model (or direct problem) and its solution that provides synthetic concentrations and states the so-called source-receptor relation. In this step, a series of considerations concerning the dispersion model must be made, such as the physical-chemical processes involved and the techniques used to solve the resulting partial differential equation (PDE) problem.

The second step is the set up of an inverse problem method that can be based on deterministic or stochastic techniques. In the deterministic set of solutions, in general, an objective function that relates observed and calculated concentrations must be minimized, and such minimization can be performed by a series of techniques, including gradient-based methods, meta-heuristic optimization tools or both. For more details, see Albani *et al.* (2020); Hutchinson *et al.* (2017) and references therein.

The stochastic class of solutions is, in general, based on Bayesian inference that considers all the observed and unknown quantities as random variables, and can make use of Monte Carlo Markov Chain (MCMC) methods to obtain samples for the unknown quantities, exploring the so-caled full conditional distributions (Gamerman and Lopes, 2006).

The main advantage of deterministic tools is their computational efficiency, whereas, the Bayesian inference introduces naturally the uncertainties underlying the concentration measurements and the dispersion model.

In the context of estimation of atmospheric releases, both techniques were recurrently used. For example, to estimate emission sources, Albani and Albani (2019, 2020); Albani *et al.* (2020) use deterministic tools, whereas Addepalli *et al.*

(2011); Hosseini and Stockie (2017); Wade and Senocak (2013) use stochastic methods.

The main difficulties arising in the estimation of atmospheric releases stem from both, the direct and the inverse problems. In the direct problem, we can mention the tricky hypotheses concerning all the approximations needed to build an efficient and accurate computational model for the dispersion problem. In the inverse problem there are the uncertainties in the measurement of concentrations, inaccuracies in the dispersion modeling, as well as physical phenomena like diffusion that may lead to a so-called ill-posed problem, i.e, the inverse problem may not have a solution, the solution may not be unique, or it can be sensitive to small perturbation in the data. All these issues and its intrinsic importance illustrate how difficult is to provide a solution for source identification problems and why it received much attention in the last decades.

Since the standard finite element method (FEM) is not appropriate to atmospheric flow and atmospheric dispersion simulations due to the emergence of non-physical oscillation in the solution (Albani *et al.*, 2015), in this work we apply the stabilized Galerkin Least-Square (GLS) FEM formulation proposed in Hughes *et al.* (1989) to solve the dispersion problem. The estimation of the source location and strength is performed by an adaptive Monte Carlo Markov Chain (MCMC) algorithm inspired in the state dependent method from Roberts and Rosenthal (2009). We estimate also the so-called precision of the concentration measurements simultaneously to the source parameters by performing Metropolis in Gibbs steps Gamerman and Lopes (2006); Müller (1994); Robert *et al.* (2010). Combining an adaptive MCMC algorithm with the precision estimation potentially improves the accuracy of estimation and the computational efficiency of the proposed technique.

It is worth mentioning that, due to the linearity of the source-receptor relation, we replace the original dispersion PDE problem by an adjoint state one that is numerically solved only once for each sensor, turning the Bayesian approach computationally appealing. Moreover, due to the FEM properties, the GLS formulation allows the application of the proposed source identification methodology to a broad range of atmospheric conditions and geometry settings.

2. SOURCE IDENTIFICATION MODELING

This section presents the proposed source identification model, that is composed by the dispersion model defining the source-receptor relation and by a Bayesian inference framework that is used to estimate the source location and strength based on observed concentrations.

2.1 Adaptive MCMC Algorithm

Given a set of concentrations denoted by the n-dimensional vector C^{obs}, we want to estimate its origin and the amount of pollutant released, represented by the 4-dimensional vector $\mathbf{v}_s = (x_s, y_s, z_s, Q_s)$, where (x_s, y_s, z_s) represents the source location and Q_s the source strength. The source-receptor relation established by the numerical solution of the dispersion problem in Eq (10)–(12) can be defined as

$$C(\mathbf{v}_s) = C^{\text{obs}}, \tag{1}$$

where $C(\mathbf{v}_s)$ denotes the concentrations evaluated by the numerical scheme at the sensors locations.

However, due to a series of uncertainties underlying the concentration measurements and the dispersion problem modeling, a relation like the one in Eq. (1) may not hold in general. Thus, since the observed quantities are non-negative and to turn their discrepancy symmetric, we assume that $C(\mathbf{v}_s)$ and C^{obs} are related through the following equation:

$$\ln\left(C(\mathbf{v}_s)\right) - \ln\left(C^{\text{obs}}\right) = \varepsilon, \tag{2}$$

where ε denotes a n-dimensional normal-distributed random noise, with mean $\mathbf{0}$ and covariance matrix $p^{-1}I$, where p is an unknown positive constant so-called precision. So, we denote $\varepsilon \sim N(\mathbf{0}, p^{-1}I)$. Therefore, the set of unknown variables is p and $\mathbf{v}_s$. Notice that the observed concentrations are independent.

By Eq. (2) and the distribution of ε, we can define the likelihood function as

$$P\left(C^{\text{obs}}\,|p, \mathbf{v}_s\right) \propto p^{\frac{n}{2}} \exp\left(-\frac{p}{2}\left\|\ln\left(C(\mathbf{v}_s)\right) - \ln\left(C^{\text{obs}}\right)\right\|_{\ell_2}^2\right). \tag{3}$$

The unknowns p and $\mathbf{v}_s$ have independent prior distributions, where p has distribution $\Gamma\left(\frac{n_0}{2}, \frac{d_0}{2}\right)$ and $\mathbf{v}_s$ has a uniform distribution in the following set:

$$[x_{\min}, x_{\max}] \times [y_{\min}, y_{\max}] \times [z_{\min}, z_{\max}] \times [Q_{\min}, Q_{\max}].$$

The full conditionals of p and $\mathbf{v}_s$ are given by:

$$P\left(p\middle|\mathbf{v}_s, C^{\text{obs}}\right) \propto P\left(C^{\text{obs}}|p, \mathbf{v}_s\right) P(p), \tag{4}$$

$$P\left(\mathbf{v}_s\middle|p, C^{\text{obs}}\right) \propto P\left(C^{\text{obs}}|p, \mathbf{v}_s\right) P(\mathbf{v}_s), \tag{5}$$

where $P(\mathbf{v}_s)$ and $P(p)$ denote the prior densities of $\mathbf{v}_s$ and p, respectively. Since $P(p)$ is a Gamma density and the likelihood function is a Gaussian density, it follows that the full conditional of p is proportional to a Gamma density, so, the random variable p given $\mathbf{v}_s$ and C^{obs} has distribution $\Gamma\left(\frac{\tilde{n}}{2}, \frac{\tilde{d}}{2}\right)$, where $\tilde{n} = n_0 + n$ and $\tilde{d} = d_0 + \| \ln(C^{\text{obs}}) - \ln(C(\mathbf{v}_s))\|^2_{\ell_2}$, which can be easily sampled. On the other hand, it is not possible to obtain samples of the full conditional of $\mathbf{v}_s$ directly. In order to find samples of p and $\mathbf{v}_s$, we apply a Monte Carlo Markov chain (MCMC) algorithm that is inspired in the adaptive state-dependent scaling method from Roberts and Rosenthal (2009) and uses the steps provided by the Metropolis in Gibbs algorithm (Gamerman and Lopes, 2006; Müller, 1994; Robert *et al.*, 2010). Algorithm 1 presents the pseudo-code summarizing the proposed method.

Algorithm 1 MCMC algorithm with adaptive steps.

procedure MCMC ALGORITHM
  $j = 0$
  $p^j = p, \mathbf{v}_s^j = \mathbf{v}_s$
  while $j \leq$ MaxIter **do**
    Draw $\mathbf{u} \sim N(\mathbf{v}_s^j, Z)$
    Evaluate $\tilde{n}$ and $\tilde{d}$
    Draw $p^{j+1} \sim \Gamma\left(\dfrac{\tilde{n}}{2}, \dfrac{\tilde{d}}{2}\right)$
    Evaluate $P\left(\mathbf{v}_s^j\middle|p^{j+1}, C^{\text{obs}}\right)$ and $P\left(\mathbf{u}\middle|p^{j+1}, C^{\text{obs}}\right)$
    Evaluate $\beta = \min\left(1, \dfrac{P\left(\mathbf{u}\middle|p^{j+1}, C^{\text{obs}}\right)}{P\left(\mathbf{v}_s^j\middle|p^{j+1}, C^{\text{obs}}\right)}\right)$
    Draw $l \sim U[0,1]$
    if $l < \beta$ **then**
      Accept: $\mathbf{v}_s^{j+1} = \mathbf{u}$
    else
      Reject: $\mathbf{v}_s^{j+1} = \mathbf{v}_s^j$
    end if
    $j = j + 1$
  end while
end procedure

The covariance matrix Z in the Gaussian random walk distribution is defined to turn the algorithm adaptive and is set as follows:

$$[Z]_{ii} = \nu_i \text{ and } [Z]_{ij} = 0, \text{ if } i \neq j,$$

with $(\nu_1, \nu_2, \nu_3, \nu_4) = c^j(l_x, l_y, l_z, l_Q)$, $c^j = 2^\alpha c^{j-1}$. As in Roberts and Rosenthal (2009), after sets of 100 steps in the MCMC algorithm, the exponent α assumes the value 1, if the Metropolis acceptance ratio was larger than 23%, i.e., if the proposed value is accepted 23 times or more, and -1 otherwise. The quantities l_x, l_y, l_z, and l_Q are the lengths o the intervals where the variables x, y, z, and Q may vary in the computational domain.

2.2 Dispersion model

The numerical concentration in the previously described Algorithm (1) is obtained as the solution of the following Partial Differential Equation (PDE),

$$\mathbf{u} \cdot \nabla C - \nabla \cdot (\mathbf{K}\nabla C) = Q\delta(x - x_s)\delta(y - y_s)\delta(z - z_s), \tag{6}$$

for any spatial position (x, y, z) over the computational domain Ω. The vector $\mathbf{u}$ stands for the wind field and the tensor $\mathbf{K}$ is a diagonal 3×3 matrix, with diagonal components K_x, K_y and K_z representing the turbulent diffusion in the x, y

and z directions respectively. Further, (x_s, y_s, z_s) corresponds to the source coordinates, Q stands for the emission rate and δ is the Dirac delta distribution. To complete the dispersion model in Eq. 6 the following boundary conditions are considered:

$$\mathbf{n} \cdot \nabla C = 0. \tag{7}$$

The vector **n** stands for the outward normal on the boundaries of Ω at $z = z_0$ and $z = h$, and

$$C = 0 \quad \text{elsewhere.} \tag{8}$$

In this work, z_0 (m) represents the surface roughness length and h (m), the ABL height. Eq. (7) assumes no flux across the corresponding boundaries and Eq. (8) indicate that the pollutant concentration goes to zero far away from the source of emission.

A usual procedure in source identification problems is to substitute Eq. (6) by an adjoint equation. This procedure is performed to avoid solving the dispersion model in Eqs. (6)-(8) at each step of the Markov chain algorithm. Thus, following Pudykiewicz (1998), we replace this original PDE problem by an adjoint PDE. The adjoint PDEs need to be solved only once, for each concentration measurement. Such a procedure results on a significant economy in the computational time.

Considering the linearity of Eq. (6), it is possible to establish a direct relationship among the source and the sensors following to the adjoint state PDE. Denoting the observed concentration at the kth sensor by $C^{obs}(x_k, y_k, z_k)$, it follows that

$$C^{obs}(x_k, y_k, z_k) = \sum_{j=1}^{n} \int_{\Omega} C_k^* \mathbb{S}_j d\Omega = \sum_{j=1}^{n} \langle C_k^*, \mathbb{S}_j \rangle, \tag{9}$$

wherein C_k^* represents the solution of the following adjoint-state PDE (Mamonov and Tsai, 2013):

$$-\mathbf{u} \cdot \nabla C^* - \nabla \cdot (\mathbf{K} \nabla C^*) = \mathbb{S}_k, \tag{10}$$

wherein $\mathbb{S}_k$ represents the kth sensor, defined as

$$\mathbb{S}_k(x, y, z, t) = \delta(x - x_k)\delta(y - y_k)\delta(z - z_k),$$

where (x_k, y_k, z_k) is the spatial coordinate of the kth sensor, considering a set of n_s sensors. The boundary conditions to Eq. (10) are as follows:

$$\mathbf{n} \cdot \nabla C^* = 0 \quad \text{on the boundaries of } \Omega \text{ at } z = z_0 \text{ and } z = h, \tag{11}$$

and

$$C^* = 0 \quad \text{elsewhere.} \tag{12}$$

Therefore, they are quite similar to (7)-(8). Atmospheric variables may undergo drastic changes in time affecting the pollutant dispersion. The atmospheric dispersion is described according to an advection-diffusion equation. Depending on the meteorological conditions, the atmosphere can be advection or diffusion-dominated. To avoid possible non-physical oscillations usual in the standard FEM, we solve the adjoint-state PDE (10) the Galerkin-Least/Squares formulation from Hughes *et al.* (1989). We did not present this formulation in this work, since it can be found in Albani and Albani (2019).

2.3 Test problem

We now give a brief description of the problem to be solved in this work. We try to identify the spatial coordinates (x_s, y_s, z_s) and emission rate (Q) from the single source tracer experiment of Copenhagen Gryning (1981); Gryning and Lyck (2002). The real values of (x_s, y_s, z_s) and Q are given from the experiment report, as well as meteorological and concentration data. The experiment report Gryning and Lyck (2002) describes in details all the experimental campaign. In this work, we give only the information necessary to reproduce computationally the experiment.

The tracer gas SF_6 was released without buoyancy from a 115 m a tower, under neutral and unstable atmospheric conditions. The meteorological data were measured by instruments positioned at different heights of the tower. Then, the tracer was collected 2-3 m above the ground level over a net of sensors located radially 2, 4, and 6 km from the release. The period of release was 11:47 am to 1:18 pm. Then, three consecutive 20 min averaged tracer concentrations were measured, allowing for a total sampling time of 1 hour.

In this work, we consider two consecutive 20 minutes averaged concentration measurements in the time interval ranging from 12:13 pm to 12:53 pm (runs 1 to 2) resulting in a total sampling time of 1 hour considering the experiment performed on October 19th, 1978. The roughness length was estimated at 0.6 m.

Considering the flatness of the terrain over the experimental site, we apply parametric profiles for the wind intensity and vertical turbulent diffusion (6) proposed by Ulke (2000). This procedure avoid to solve the Navier-Stokes equations to obtain the wind field to necessary to solve the dispersion model (10).

The parametric profiles are functions of the frictional velocity (u_*), the Monin-Obukhov length (L), the ABL height (h), and the vertical coordinate z. Thus, the vertical turbulent diffusion coefficient is given, for unstable conditions ($h/L < 0$), by

$$K_z(z) = \kappa u_{*0} h \left(\frac{z}{h}\right)\left(1 - \frac{z}{h}\right)\left(1 - 22\frac{h}{L}\frac{z}{h}\right)^{1/4}, \tag{13}$$

and the wind intensity is

$$u = \frac{u_{*0}}{\kappa}\left\{\ln\frac{z}{z_0} + \ln\left[\frac{(1+\mu_0^2)(1+\mu_0)^2}{(1+\mu^2)(1+\mu)^2}\right] + 2(\arctan(\mu) - \arctan(\mu_0)) + \frac{2L}{33h}[\mu^3 - \mu_0^3]\right\}, \tag{14}$$

with

$$\mu = \left(1 - 22\frac{h}{L}\frac{z}{h}\right)^{1/4} \qquad \text{and} \qquad \mu_0 = \left(1 - 22\frac{h}{L}\frac{z_0}{h}\right)^{1/4}.$$

We assume that the other diffusion components satisfy $K_x = K_y$, and set to the value $K_x = 50$ m^2/s, which is commonly applied for unstable conditions Arya (2001).

Considering the experiment performed on October 19th, 1978, the meteorological parameters are given by $h = 1120$ m, $u_* = 0.39$ m/s and $L = -108$ m. During the sampling time interval, $\theta = 290°$. Besides, the spatial coordinates of the source is $(0, 0, 115)$m and the source strength was 3.2g/s.

3. RESULTS

This section presents a experimental evaluation of the Algorithm (1) using one run of the Copenhagen experimental dataset (Gryning, 1981; Gryning and Lyck, 2002). The numerical solution of the dispersion problem was already evaluated in the previous works Albani and Albani (2019); Albani *et al.* (2020) with the same dataset, so we omit it here. The uniform prior density of $\mathbf{v}_s$ is defined based on the experimental setup (sensors spatial distribution) and the wind direction, in order to reduce the search region and let the algorithm. We design straight lines in the xy-plane that pass through the sensors located at the edge of the first and third arcs of used sensors. Moreover, we assume that the x-coordinate must be restricted to $[-1000, 1000]$ m. The resulting region where the coordinates x and y are allowed to vary is the trapezoidal-like region depicted in Figure 1. The coordinate z and Q can vary in the intervals $[0.6, 1120]$ m and $[0, 30]$ g/s, respectively.

Algorithm 1 is initialized with a uniformly-distributed sample for $\mathbf{v}_s$, with x and y given in the region in Figure 1, and (z, Q) in $[0.6, 1120] \times [0, 30]$. The precision p is generated by the Gamma distribution $\Gamma(\frac{n_0}{2}, \frac{d_0}{2})$ with $n_0 = 10^{-3}$ and $d_0 = 10^{-3}$. The Markov Chain is composed by 50 thousand states, where the first 10 thousand are discarded as the burn-in set, and, from the remaining 40 thousand states, we select 800 states using a step-size of 50 states. The histograms as well as the plots of the resulting chains for x, y, z, Q, and p can be found in Figures 2–3. The corresponding summary statistics is shown in Table 1.

The calibration procedure is performed in the following two steps:

1. We let Algorithm 1 to draw proposals for p and $\mathbf{v}_s$, but, the chains of z_s and Q_s were the only that stabilized.

2. We used samples from the chains of z_s and Q_s to fix their values.

3. With z_s and Q_s fixed, we estimate the remaining parameters, namely, p, x, and y.

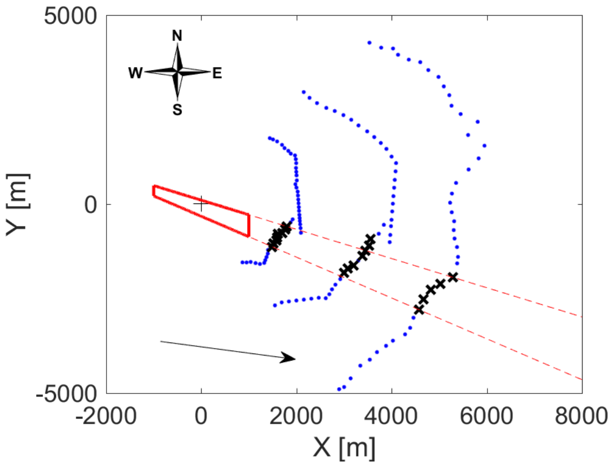

Figure 1. The trapezoidal-like region (delimited by solid lines) is where the x and y coordinates of the source must be searched. The source true location is given by the cross, the dots represent all the sensors, and the x-symbols represent the used sensors.

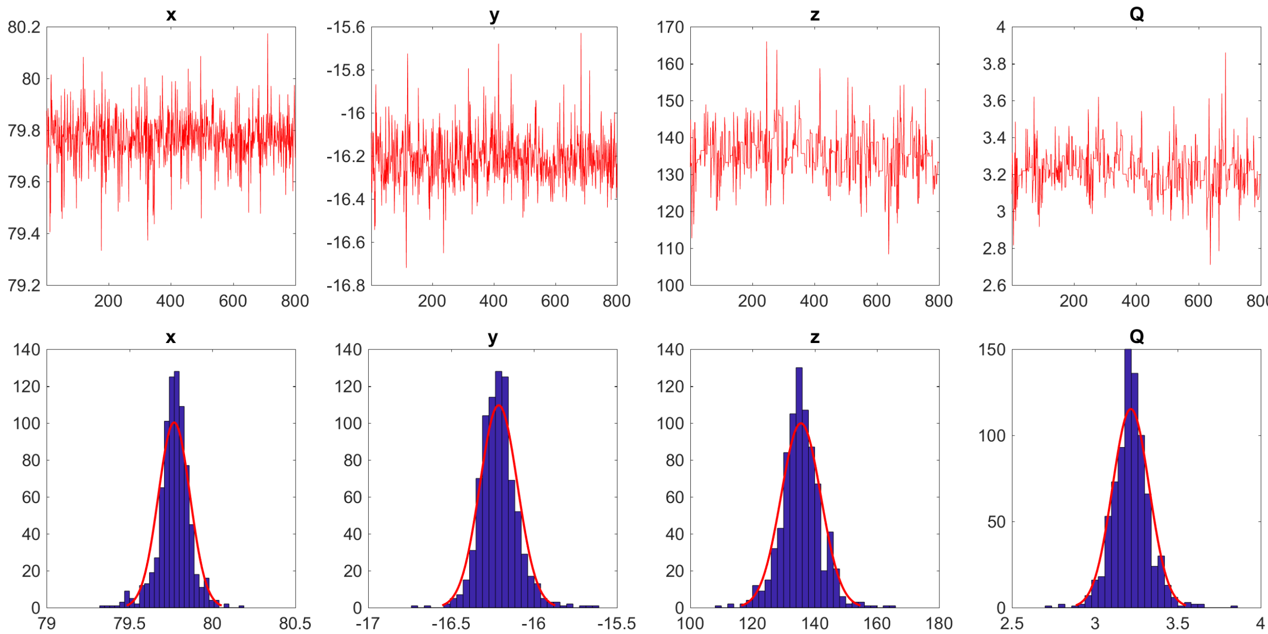

Figure 2. States (top row) and histograms (bottom row) of the parameters x_s, y_s, z_s, and Q_s.

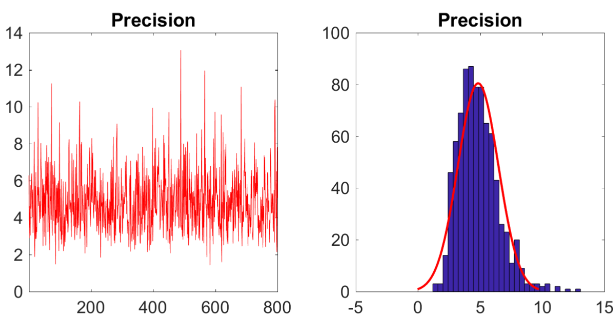

Figure 3. States and histogram of the precision p.

The samples of z_s and Q_s contain their corresponding ground truth values. Although the samples of x_s and y_s do not contain their ground truth values, the sample set is close the corresponding true values, presenting an accuracy similar to the observed using deterministic techniques with more sophisticate likelihood or data misfit functions as in Albani and Albani (2019); Albani *et al.* (2020). Such accuracy may be due to the simultaneous estimation of the precision p that

Table 1. True values (True) and summary statistics of the chains, i.e., minimum value (Min.), the first quartile (Q1), the median value (Median), the third quartile (Q3), the maximum value (Max.) and the value of the Gelman-Rubin convergence test (GR Test) for each variable.

Parameter	True	Min.	Q1	Median	Q3	Max.	GR Test
x_s [m]	0	79.3	79.7	79.8	79.8	80.2	1.00
y_s [m]	0	-16.7	-16.3	-16.2	-16.2	-15.6	1.00
z_s [m]	115	108	132	135	139	166	1.05
Q_s [g/s]	3.2	2.71	3.16	3.22	3.28	3.86	1.05
p	-	1.44	3.70	4.66	5.76	13.1	1.00

addresses the uncertainties underlying the concentration measurements. It is worth mentioning that, the computational cost of this estimation procedure is similar to deterministic techniques due to the numerical solution of the dispersion problem, that must be run only once and before the initialization of Algorithm 1. In addition, the use of an adaptive strategy in the MCMC algorithm may also have contributed to save computational time in the reconstructions of the parameters (Roberts and Rosenthal, 2009).

4. CONCLUSIONS

The present article proposes an inversion methodology based on Bayesian inference to estimate emission sources in the ABL. The dispersion problem was solved by a GLS/FEM formulation combined with parametric profiles for the wind intensity and the vertical diffusion allowing the introduction of relevant physical information that potentially improves the so-called source-receptor/sensor relation (Albani and Albani, 2019; Albani *et al.*, 2020). An accurate solution of the direct problem is essential to improve the inversion methodology (Albani and Albani, 2019; Hosseini and Stockie, 2017). Besides, considering the linearity of the source-receptor relation, the dispersion problem was solved only once for each sensor. This procedure makes the MCMC algorithms competitive in comparison to deterministic techniques like Tikhonov-type regularization.

In the proposed Bayesian approach, the source parameters, i.e., its spatial location and strength, and the precision are estimated simultaneously using a Metropolis in Gibbs algorithm with adaptive steps. The Gibbs step provides a sample for the precision, whereas the Metropolis step gives a proposal for the source parameters samples. The adaptive step is performed in the search for the source parameters and takes into consideration the size of the computational domain, as well as the acceptance ratio given by the Hastings ratio at each step, following Roberts and Rosenthal (2009). The resulting methodology provided estimations for the source parameters with a level of accuracy and computational time similar to the ones observed in Albani and Albani (2019); Albani *et al.* (2020) obtained with Tikhonov-type regularization and intricate likelihood or merit functions.

The estimation procedure was also broken up into two main steps. In the first one, we provide estimates for z and Q, then, holding z and Q fixed, estimates for x and y were found.

The prior density used in the estimation accounted for the wind direction and the experimental setup, i.e., the sensors distribution, reducing considerably the search region, also helping to improve the estimation.

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6. REFERENCES

Addepalli, B., Sikorski, K., Pardyjak, E. and Zhdanov, M., 2011. "Source characterization of atmospheric releases using stochastic search and regularized gradient optimization". *Inverse Probl. Sci. Eng.*, Vol. 19, No. 8, pp. 1097–1124. doi:10.1080/17415977.2011.589901.

Albani, R. and Albani, V., 2020. "An Accurate Strategy to Retrieve Multiple Source Emissions in the Atmosphere". *Atmos. Environ.*, Vol. 233, p. 117579. doi:10.1016/j.atmosenv.2020.117579.

Albani, R., Albani, V. and Silva Neto, A., 2020. "Source characterization of airborne pollutant emissions by hybrid metaheuristic/gradient-based optimization techniques". *Environ Pollut.*, Vol. 267, p. 115618. doi: https://doi.org/10.1016/j.envpol.2020.115618.

Albani, R. and Albani, V., 2019. "Tikhonov-Type Regularization and the Finite Element Method Applied to Point Source Estimation in the Atmosphere". *Atmos. Environ.*, Vol. 211, pp. 69–78. doi:10.1016/j.atmosenv.2019.04.063.

Albani, R., Duda, F.P. and Pimentel, L., 2015. "On the modeling of atmospheric pollutant dispersion during a diurnal cycle: A finite element study". *Atmos. Environ.*, Vol. 118, pp. 19–27. doi:10.1016/j.atmosenv.2015.07.036.

Arya, S.P., 2001. *Introduction to Micrometeorology*. Academic Press.

Gamerman, D. and Lopes, H.F., 2006. *Markov chain Monte Carlo: stochastic simulation for Bayesian inference*. CRC Press.

Gryning, S.E., 1981. "Elevated source SF_6 - tracer dispersion experiments in the Copenhagen area." Technical report, Risø-R-446, Risø Nacional Laboratory, 187 pp.

Gryning, S.E. and Lyck, E., 2002. "The Copenhagen tracer experiments: Reporting of measurements". Technical Report 1054, Technical University from Denmark, Denmark. Forskningscenter Risoe.

Hosseini, B. and Stockie, J., 2017. "Estimating airborne particulate emissions using a finite-volume forward solver coupled with a Bayesian inversion approach". *Computers and Fluids*, Vol. 154, pp. 27–43. doi: https://doi.org/10.1016/j.compfluid.2017.05.025.

Hughes, T., Franca, L. and Hulbert, G., 1989. "A new Finite Element Formulation for Computational Fluid Dynamics: VIII. The Galerkin/Least-Square Method for Advective-Diffusive Equations". *Comput. Methods Appl. Mech. Engrg.*, Vol. 73, pp. 173–189. doi:10.1016/0045-7825(89)90111-4.

Hutchinson, M., Oh, H. and Chen, W., 2017. "A review of source term estimation methods for atmospheric dispersion events using static or mobile sensors". *Information Fusion*, Vol. 36, pp. 130–148.

Mamonov, A. and Tsai, Y.H.R., 2013. "Point source identification in nonlinear advection-diffusion-reaction systems". *Inverse Problems*, Vol. 29, No. 3, p. 035009. doi:10.1088/0266-5611/29/3/035009.

Müller, P., 1994. "Metropolis based posterior integration schemes". In *Numerical Recipes in Fortran (2nd Edition*. Citeseer.

Pudykiewicz, J., 1998. "Application of adjoint tracer transport equations for evaluating source parameters". *Atmos. Environ.*, Vol. 32, No. 17, pp. 3039–3050. doi:10.1016/S1352-2310(97)00480-9.

Robert, C.P., Casella, G. and Casella, G., 2010. *Introducing Monte Carlo Methods with R*, Vol. 18. Springer.

Roberts, G.O. and Rosenthal, J.S., 2009. "Examples of adaptive mcmc". *J. Comput. Graph. Statist.*, Vol. 18, No. 2, pp. 349–367.

Ulke, A.G., 2000. "New turbulent parameterization for a dispersion model in the atmospheric boundary layer". *Atmos. Environ.*, Vol. 34, pp. 1029–1042.

Wade, D. and Senocak, I., 2013. "Stochastic reconstruction of multiple source atmospheric contaminant dispersion events". *Atmos. Environ.*, Vol. 74, pp. 45–51. doi:10.1016/j.atmosenv.2013.02.051.

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