21st International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes 27-30 September 2022, Aveiro, Portugal

Source characterisation of large-scale urban fires by inverse modelling

Emilie Launay^{1,2}, Virginie Hergault¹, Marc Bocquet², Joffrey Dumont Le Brazidec², Lamisse Sadeq¹, and Yelva Roustan²

 1 Laboratoire Central de la Préfecture de Police, Paris, France 2 CEREA, École des Ponts and EDF R&D, Île-de-France, France

Abstract:

Past large-scale fires in urban areas have highlighted the need to develop means of assessing the risks posed by smoke plumes to the population and the environment. One of the challenges is to quickly provide the authorities with information on the areas impacted by the plume and the pollutant concentration levels to which people may have been exposed. We present in this work the development of inverse modelling methods to retrieve the source term of a large-scale fire by assimilation of in-situ pollutant concentration measurements. A semi-Bayesian method and a Markov Chain Monte Carlo (MCMC) Bayesian method are considered for the characterisation of the source, noticeably the emission height, linked to the plume rise phenomenon, which is an important parameter to assess the impact in the fire vicinity. These inverse methods are applied within an Observing System Simulation Experiment (OSSE) corresponding to the Notre-Dame Cathedral fire in 2019 and a real case study corresponding to a large warehouse fire that occurred in Aubervilliers near Paris in 2021.

Key words: Inverse modelling, Semi-Bayesian method, Bayesian method, MCMC sampling, PMSS, Source term

Introduction

Large-scale fires in France, such as the recent fires in 2019 at the Lubrizol company warehouse and at Notre-Dame de Paris cathedral, have highlighted the need to develop means to estimate the health and environmental risks associated with this type of accident (van Geen et al., 2020). If measurements of concentrations in the atmosphere are available, it becomes interesting to use an inverse modelling method based on the joint use of these measurements and a dispersion model to characterise the source term. This approach has been widely used at large scale (for example in Winiarek et al., 2012), and, to a lesser extent at urban scale (Nguyen and Soulhac, 2016; Tilloy et al., 2013) but had little application to the dispersion of a smoke plume in a floating release situation.

In the Paris urban area, the Laboratoire Central de la Préfecture de Police (LCPP) aims to deploy a number of devices for measuring pollutants and tracers of combustion smoke during a fire. The focus is on estimating the pollution to which the population are likely to be or have been exposed. Subsequently, the application of an atmospheric dispersion model within the framework of a data assimilation system should provide a source characterisation and a finer estimate of the concentration levels at locations of interest. The dispersion model used is the Parallel Micro Swift Spray (PMSS) model developed by Aria Technologies. This is a suite of models where the Swift model first diagnoses the atmospheric flow taking as input data meteorological database from the AROME model of Météo-France at \sim 2.5 km resolution, a topography database of the National Institute of Geographic and Forest Information (IGN), and the CORINE Land Cover (CLC) database. Next, the Spray model uses the output data of the Swift model and descriptive parameters of the smoke source to perform the computation of the concentration and deposition fields with a Lagrangian approach where each particle represents a fixed amount of pollutant mass.

Methodology

The inverse methods applied to retrieve the smoke source term parameters are i) maximum a posteriori (MAP) under positive constraint and parametric estimation by Generalised Crossed Validation (GCV) and ii) a Bayesian sampling method relying on the Markov Chain Monte Carlo (MCMC) algorithm to retrieve the probability density functions associated to the parameters. The inversion procedure is carried out first by a direct modelling of the atmospheric dispersion of pollutants to construct the **H** (source-receptor) matrix describing the relationship, assumed to be linear, between the N_{obs} observed concentrations and the N_{par} inverted source term parameters, and secondly by applying a parametrisation to the inverse methods implemented (Carrassi et al., 2022). In our case, both methods are related to Bayes' formula (1) with $\mathbf{x} \in \mathbb{R}^{N_{par}}$ the set of variables of interest that characterise the source and $\mathbf{y} \in \mathbb{R}^{N_{obs}}$ the set of available observations:

$$\underbrace{p(\mathbf{x}|\mathbf{y})}_{\text{a posteriori}} = \frac{\underbrace{p(\mathbf{y}|\mathbf{x})}_{p(\mathbf{y})} \underbrace{p(\mathbf{x})}_{p(\mathbf{x})}}{\underbrace{p(\mathbf{y})}_{\text{evidence}}}.$$
(1)

A link between the two methods exists by considering Gaussian probability distributions to describe the prior (2a) and the likelihood (2b):

$$\mathbf{x} \sim \mathcal{N}(\mathbf{x_b}, \mathbf{B}): \quad p(\mathbf{x}) = \frac{1}{b^{N_{par}/2} \sqrt{(2\pi)^{N_{par}}}} e^{-\frac{1}{2} \frac{(\mathbf{x} - \mathbf{x_b})^2}{b}}, \tag{2a}$$

$$\mathbf{y}|\mathbf{x} \sim \mathcal{N}(\mathbf{H}\mathbf{x}, \mathbf{R}): \quad p(\mathbf{y}|\mathbf{x}) = \frac{1}{r^{N_{obs}/2}\sqrt{(2\pi)^{N_{obs}}}}e^{-\frac{1}{2}\frac{(\mathbf{y}-\mathbf{H}\mathbf{x})^2}{r}}, \tag{2b}$$

and by minimising only over the variable **x**, with $\mathbf{R} = r \operatorname{Id}^{N_{obs}}$ the covariance matrix linked to the model error, $\mathbf{B} = b \operatorname{Id}^{N_{par}}$ the covariance matrix linked to the prior error, and $\mathbf{x}_{\mathbf{b}} \in \mathbb{R}^{N_{par}}$ the source term estimation. With the semi-Bayesian approach, the objective is to find the maximum probability of the a posteriori which corresponds to the minimum with respect to **x** of the deterministic cost function (3) (Hansen, 2010):

$$\mathcal{J}(\mathbf{x}) = (\mathbf{y} - \mathbf{H}\mathbf{x})^{\top} (\mathbf{y} - \mathbf{H}\mathbf{x}) + \lambda^2 (\mathbf{x} - \mathbf{x}_{\mathbf{b}})^{\top} (\mathbf{x} - \mathbf{x}_{\mathbf{b}}),$$
(3)

where λ is determined through the Generalised Cross Validation method. The Limited-Memory Broyden– Fletcher–Goldfarb–Shanno with boundaries algorithm (L-BFGS-B) is used to solve the problem by gradient descent. The positive constraint of the source term is enforced through the bounds.

With the Bayesian approach, the objective is to reconstruct the a posteriori distribution by Monte Carlo sampling using the popular Metropolis-Hastings algorithm (Hastings, 1970). For a number of iterations, several states \mathbf{x} are proposed, and are either accepted or rejected given a random component, a transition probability between the states and the detailed-balance principle (4):

$$P_{\mathbf{y}}(\mathbf{x}_{new}|\mathbf{x}_{old})P_{\mathbf{y}}(\mathbf{x}_{old}) = P_{\mathbf{y}}(\mathbf{x}_{old}|\mathbf{x}_{new})P_{\mathbf{y}}(\mathbf{x}_{new}).$$
(4)

To ensure the positivity of the source term, a folded-normal distribution is considered for the transition probability. The resulting Markov chain consists of all the accepted states and allows to sample from the target distribution $P_{\mathbf{y}}$: $\mathbf{x} \to p(\mathbf{x}|\mathbf{y})$.

Synthetic case: application to Notre-Dame de Paris cathedral 2019 fire

A first application is considered in order to validate the implementation of the inverse methods and to have a first view of the inversion results in a case where the synthetic observations approximate the real conditions to which the investigation teams would have been subjected. In Paris, Notre-Dame Cathedral caught fire on April 15, 2019 around 17:00 UTC. The fire caused significant particulate pollution on an urban scale due to the lead contained in the built structure (Vallée et al., 2021). A study made by the National Institute of Risks (INERIS) considers two sources: the Cathedral spire which burned during the first hour and the frame during the three hours of the fire's fully developed phase (INERIS, 2019). Four

tracers are considered to represent different sizes of lead monoxide particles (with aerodynamic diameter of 1.5, 15, 30 and 50 μ m) for a total of 138 kg of lead monoxide emitted during the fire. The source term considered is defined according to the fully developed phase of the fire, the sources (frame, spire) and a particle size distribution. Due to the lack of measurements during the fire, synthetic observations are generated corresponding to an operational situation of teams deployment on site: measurements done between 1 km and tens of kilometres from the source in the wind direction and considering time deployment of the teams. The meteorological analyses and the source term formulated in the INERIS report are used to construct these observations. The meteorological forecasts are considered to build the H matrix via direct modelling. The discrepancies between meteorological forecasts and analyses allow to generate a typical model error within the inverse problem. Both MAP under positive constraint method and MCMC Metropolis-Hastings algorithm were used to perform a sensitivity analysis to the configuration of the inversion.

	scenario description	MNGE
sampling strategy	fixed location, full temporal coverage	0.82
	variable location, full temporal coverage	0.59
a priori	null	0.59
	uniform emission rate (5 kg/h)	0.45
	INERIS source term	0.26

Table 1: MAP results of the sensitivity study, using meteorological analyses to generate synthetic observations. MNGEis the mean normalised gross error between the inverted source term parameters and the INERIS estimate. The scoresprovided concern the PbO_{d15}. The sampling strategy sensitivity study assumes a null a priori. The a priori sensitivitystudy assumes a variable location and full temporal coverage sampling strategy.

Firstly, the sensitivity study compares a fixed location sampling strategy (on the Eiffel Tower) to a mobile location sampling strategy (relay of two teams). As a result, sampling strategy with spatio-temporal coverage helps to get closer to the expected solution (**Table** 1). Indeed, more information is provided through the observation by the variable location and full temporal coverage strategy than the fixed location. Secondly and unsurprisingly, knowledge, even partial, of the prior gives better scores on the statistical indicators for error (**Table** 1). The weighting of the prior is driven by the lambda estimate (via the GCV) which gives it sufficient importance to be sensitive. Additionally, a small change in wind direction caused a typical inverse modelling error also visible through the largely positive MNGE statistical indicator.

Real case: application to a large warehouse fire in Aubervilliers, near Paris

A second application is considered: the fire of a tool warehouse that took place on April 16, 2021 in Aubervilliers, near Paris (Figure (1a)). The fire started around 3:30 UTC, and the times of the different



Figure 1: Information on Aubervilliers's fire. (1a) Photo of the Aubervilliers warehouse smoke plume on April 16, 2021. Source: Internet. (1b) Observation map: fire (in red), distribution of PM measurement points carried out by the LCPP (in green), Airparif stations (in blue), and measurement points with an abnormal PM10 concentration peak (in orange).

phases of this fire were assessed after discussion with the firefighters and study of drone images taken during the fire. It is estimated that the fire experienced its fully developed phase between 4:30 UTC and 6:30 UTC, was brought under control around 7:30 UTC, and was contained by 8:30 UTC. A first approximation of the source term is made by estimating the heat release rate (HRR) from these indications. An initial estimate of the emission height is based on photos and information given by the firefighters. Thus, five heights are sampled from 100 m to 500 m. The observations are provided by ten AirParif measurement stations located in and near Paris. Among these stations (**Figure (1b**)) five detected an abnormal concentration of PM₁₀ (greater than 120 μ g.m⁻³) during the fire.

The MCMC method is used to reconstruct the a posteriori distribution for this case, giving an evaluation of the uncertainties. For now, a choice is made on r and b through the results given by the GCV estimation (used with the MAP method): $\lambda = 0.217$, and $\lambda^2 = r/b$. Thus, in the following we will assume b = 10 and r = 0.47. With the same configurations, both MAP under positive constraint and MCMC method tend to find similar kinetics of the fire for this case. Indeed, the first results show a temporal evolution of the intensity release with a peak for the third hour of the fire which is consistent with the source term estimation: the maximum rate is found in the predominant hour of the fully developed phase of the fire.

Due to the empirical and deterministic choice of the parameter r linked to the model error and indirectly to the prior error, a sensitivity study to the a priori was carried out. As a result, the releases at the 400 m and 500 m emission heights appear very sensitive to the prior (**Figure 2**) and cannot be considered as a robust solution to the inverse problem. In contrast, the 300 m emission height stands out from the other which is consistent with smoke plume visual estimations. Indeed, the intensity release for the 300 m emission height is significantly greater than the 100 m and 200 m emission heights and also stands apart from the prior. However, the retrieved intensity release for the 300 m emission height still depends on it. An improvement of the MCMC method by considering a stochastic estimation of r, avoiding an arbitrary choice, would yield a more robust estimation of the release intensity.





(a) MCMC results assuming a 100 kg/h uniform emission rate for the a priori.

(b) MCMC results assuming a 200 kg/h uniform emission rate for the a priori.

Figure 2: MCMC's resulting a posteriori distribution for emission rate in kg/h between 5:30 UTC and 6:30 UTC and for five emission heights.

It is also possible (and recommended) to take into account the background component of the observed concentrations in the inversion. We can even distinguish this contribution, due to all other sources besides the fire, depending on whether the observations sites are representative of the urban background concentrations or of traffic proximity concentrations. The first results of background concentrations inversion obtained with the MAP method ($\sim 34 \,\mu g.m^{-3}$ for traffic stations and $\sim 25 \,\mu g.m^{-3}$ for urban background stations) are consistent with the observed conditions of the day and the usual background estimates made by AirParif ($\sim 20 \,\mu g.m^{-3}$ and $\sim 15 \,\mu g.m^{-3}$ respectively).

Conclusions

Two inverse methods have been implemented in order to characterise the intensity of the release and the emission height of smoke in case of large-scale fires.

The implementation of the maximum a posteriori under positive constraint and Markov Chain Monte Carlo methods have been validated on the synthetic case of the Notre-Dame de Paris fire. In the case of a real fire, the MCMC method provides releases estimates consistent with the source term derived in previous situations (Alp and Michalowicz, 2005; Daly et al., 2012) and with an estimate of the source term (via data transmitted by the firefighters). Also, the background concentrations can be taken into account within the inversion problem and coincides with the expected values.

For the MCMC method, the r parameter drives the uncertainties linked to the solution. More rigorously, the hyperparameter r can be incorporated into the MCMC algorithm in order to be estimated in the inversion process (Dumont Le Brazidec et al., 2021). This improvement of the implemented algorithm will be the next step in this work. The use of distributions other than Gaussian for the likelihood and the a priori is a perspective as well. For instance, the ability of log-normal statistics to process positive variables of significantly different magnitudes is a major asset.

REFERENCES

Alp, E., and R. Michalowicz, 2005: Modeling of a warehouse fire - a case study.

- Carrassi, A., M. Bocquet, J. Demaeyer, C. Grudzien, P. Raanes, and S. Vannitsem, 2022: Data Assimilation for Chaotic Dynamics, 1–42. Springer International Publishing, Cham, doi:10.1007/978-3-030-77722-7_1, URL https://doi.org/10.1007/978-3-030-77722-7_1.
- Daly, A., P. Zannetti, and T. Echekki, 2012: A combination of fire and dispersion modeling techniques for simulating a warehouse fire. *International Journal of Safety and Security Engineering*, 2, 368–380, doi: 10.2495/SAFE-V2-N4-368-380.
- Dumont Le Brazidec, J., M. Bocquet, O. Saunier, and Y. Roustan, 2021: Quantification of the modelling uncertainties in atmospheric release source assessment and application to the reconstruction of the autumn 2017 Ruthenium 106 source. *Atmos. Chem. Phys.*, 1–28, doi:10.5194/acp-2020-1129, URL https: //acp.copernicus.org/preprints/acp-2020-1129/, publisher: Copernicus GmbH.
- Hansen, P. C., 2010: Discrete inverse problems. Insight and algorithms, Vol. 7. 85–108 pp., doi:10.1137/1. 9780898718836.
- Hastings, W. K., 1970: Monte carlo sampling methods using markov chains and their applications. *Biometrika*, **57 (1)**, 97–109, URL http://www.jstor.org/stable/2334940.
- INERIS, 2019: Modélisation de la dispersion des particules de plomb du panache de l'incendie de Notre Dame. Rapport Technique. Institut National de l'Environnement Industriel et des Risques, v2 (200480-879062).
- Nguyen, C. V., and L. Soulhac, 2016: Evaluation of data assimilation method at the urban scale with the sirane model.
- Tilloy, A., V. Mallet, D. Poulet, C. Pesin, and F. Brocheton, 2013: Blue-based no 2 data assimilation at urban scale. *Journal of Geophysical Research: Atmospheres*, **118**, doi:10.1002/jgrd.50233.
- Vallée, A., E. Sorbets, H. Lelong, J. Langrand, and J. Blacher, 2021: The lead story of the fire at the notredame cathedral of paris. *Environmental Pollution*, **269**, 116140, doi:https://doi.org/10.1016/j.envpol.2020. 116140, URL https://www.sciencedirect.com/science/article/pii/S0269749120368299.
- van Geen, A., Y. Yao, T. Ellis, and A. Gelman, 2020: Fallout of lead over paris from the 2019 notre-dame cathedral fire. *GeoHealth*, **4**, doi:10.1029/2020GH000279.
- Winiarek, V., M. Bocquet, O. Saunier, and A. Mathieu, 2012: Estimation of errors in the inverse modeling of accidental release of atmospheric pollutant: Application to the reconstruction of the cesium-137 and iodine-131 source terms from the fukushima daiichi power plant (vol 117, d18118, 2012). Journal of Geophysical Research (Atmospheres), 117, 18118–, doi:10.1029/2012JD018107.