

**17th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
9-12 May 2016, Budapest, Hungary**

MODITIC INVERSE MODELLING IN URBAN ENVIRONMENTS

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Abstract: Linear inverse dispersion modelling, in particular from a single point source, is a maturing field where least square optimisation methods as well as Bayesian approaches have been adapted to solve the problem. In many studies, however, the setting is both oversimplified (flat terrain, Gaussian plume dispersion models) and the detector data generated synthetically. In the present study we bring linear inverse modelling to an urban environment (there are up to 14 buildings in the town studied) and we use detector signals from MODITIC wind tunnel experiments of the same configuration. We employ two different methods, renormalisation (Issartel et al, 2012) and a Bayesian framework, to solve the resulting inverse problem. We compare and contrast the two different methods and their results. Both methods rely on having adjoint functions for computational efficiency. In this case the adjoint fields are RANS CFD-fields.

Key words: *Inverse modelling, urban environment, linear atmospheric dispersion, Bayesian, Renormalisation*

INTRODUCTION

Over the years atmospheric dispersion models have been developed and refined to be able to cope with dispersal problems of varying, or rather increasing, complexity: the original problems were usually involving a hazardous substance that was dispersed linearly by a given meteorology over flat terrain while today the state-of-the-art cases, like those studied in the MODITIC project, handle nonlinear dispersal in built up environments. Being able to predict where a known release of a hazardous substance is carried by the wind field in order to calculate risk areas, estimate casualties and devising mitigating actions is important. These are questions that typically arise before an event has taken place, or, possibly during an event if the source of the release is known. Often the source is unknown, indeed networks of sensors are employed around critical infrastructure or soft targets to give an early warning of a developing event. That raises the natural question: can the knowledge of how a hazardous substance disperse through the atmosphere combined with the information given by the detectors allow us to deduce where the hazardous substance was released, i.e. determine the source. Enter inverse dispersion modelling. In this talk we will use two different inverse modelling techniques and apply them to a linear inverse problem set in a built up environment. We verify the methods for synthetic sensor data, showing what accuracy we can expect from the methods, and then apply the methods to sensor data generated in wind tunnel experiments.

EXPERIMENTAL SET-UP

We study two urban environments of increasing complexity: the simple array with 4 equal sized buildings, and a complex array with 14 buildings of varying sizes.

Simple array

The dimensions of the simple array, with the positions of the synchronized detectors we use for backtracking is shown in **Figure 1**.

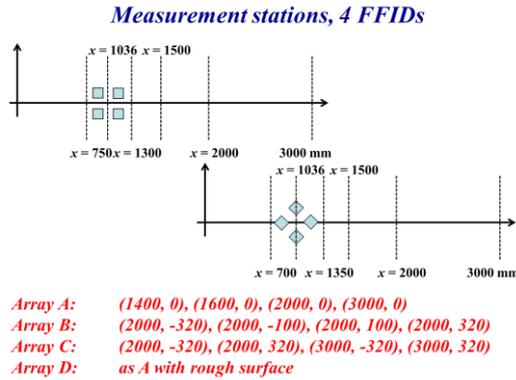


Figure 1. Sensors network (A, B, C arrangement) for the simple array cases. In each scenario 4 synchronized detectors are used to measure the concentration of the released gas. The detectors are located at the positions stated under A, B and C respectively.

The wind direction in the wind tunnel experiments is aligned with the x-axis in **Figure 1**, and as shown in the figure the simple array may be aligned at two different angles: we denote the alignment in the upper pane as “0 degrees” and the alignment in the lower pane as “45 degrees”. In each scenario four synchronized detectors were used, hence the reference 4 FFID in **Figure 1**, and we chose three different sets of locations for these detectors: we refer to these as case A, B and C. In addition to this two different source locations were available: these we denote S1 and S2, both S1 and S2 (at the origin) are located at $8H$ upwind ($= -0.88m$) in the x direction, but S1 is shifted off the x-axis by $1.5H$ ($= 0.165m$) in the +y direction. The location of S2 was chosen to be the origin of the coordinate system. The diameter of the sources is $0.1m$ (to be compared to building height and sides of $H=0.11m$). A constant release rate of $50l/min=8.33e-4 m^3/s$ was used in all scenarios.

Complex array

In the complex array there are more buildings present and there is less symmetry. The configuration also opens up for a larger number of sensible detector locations, however, still only 4 synchronized detectors were used in these scenarios. For the complex array we chose five different sets of detector configurations: these are denoted case A through to E, and these are shown together with the geometry of the complex array in **Figure 2**. Note that some detectors are located on the roof tops (cases A and C) and other are inside the street canyons (cases B, D and E).

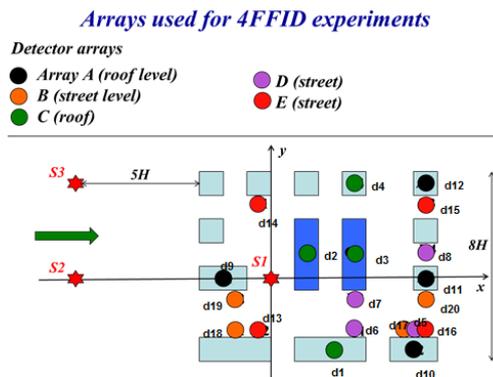


Figure 2: Configuration of the complex array. In each scenario, denoted case A through to E, 4 synchronized detectors were used to measure the concentration of the released gas. Note that some detectors are located at the roof of the buildings. Two different source locations were used, denoted S1 and S2. (There is a third source S3 indicated in the figure, but it was not used for inverse modelling).

Two different source locations were used S1 and S2. The diameter of the sources is $0.1m$. The source S1 is defined to be at the origin (see **Figure 2**) while S2 is located upwind at $x=-8H=-0.88m$ and $y=0$. S1 and

S2 are both located on the ground. As for the empty and complex array the source strength is $50\text{l}/\text{min}=8.33\text{e-}4\text{m}^3/\text{s}$.

For full details on the wind tunnel experiments that were conducted we refer to (Robins et al, 2016).

INVERSE MODELLING METHODS

There are many inverse modelling techniques for atmospheric dispersion problems, but in general there are two main classes of such methods in use: in the first one the inverse problem is considered to be a probabilistic problem and Bayes theorem is used to deduce information about the source, in the second one the problem is viewed as a deterministic problem and the source is solved for by using some optimality principle (e.g. least squares). Common for both of these classes of methods is that they rely on being able to link a hypothetical source to its sensor response (a source-sensor relationship). This source-sensor relationship is readily given by the atmospheric dispersion model if it was not for the problem of computational cost. For each hypothetical source the atmospheric dispersion model must be used to establish the desired source-sensor relationship, for a Gaussian model on flat terrain this could be doable, but in the case of complex geometry and CFD-models it is not feasible. Thus a method called adjoint plumes is used. This method initially requires a more involved mathematical derivation, but once the adjoint model is found and it only have to be solved once for each detector to establish the source-sensor relationship. As part of the MODITIC project it was shown that neutral gas release for the simple and complex array are self-adjoint (Brännvall, 2015).

Bayesian method

In the Bayesian approach to the inverse problem the source is estimated from the a posteriori probability distribution function which is obtained by calculating a likelihood function and weighing it with any a priori information that one has at hand (see e.g. (Stuart, 2010) for an introduction to general Bayesian inverse problems, and (Franklin, 1970) for an early reference). Let u be the sought input (the source), and y the observed sensor data, then the posterior distribution is given by

$$P(u | y) = \frac{P(u)P(y | u)}{P(y)}$$

where $P(u)$ is the prior distribution, $P(y | u)$ is the likelihood and $P(y)$ is the evidence – the latter is only normalising the distribution and is not required for sampling the posterior distribution. This method avoids the pitfalls of ill-conditioning which are often associated with directly inverted problems and adds the benefit of allowing uncertainties in models and measurements to be handled in a tractable fashion.

Renormalisation

Renormalization theory is a theory for data assimilation that allows reconstructing some estimated sources (Turbelin et al, 2014). It works in linear situations, where the measurements depend linearly on the source that is to be estimated. The estimated source is then a linear function of the measures, and no prior data has to be incorporated to the inputs: the experimenter does not have to guess what could be the source, nor the error of the model that has been used. The only inputs are the measurements μ and the adjoint function $a(x)$ (i.e., the values of the measurements associated to point sources).

To compute these adjoint functions, it is helpful to first compute retro-plumes and to make a post-treatment to eventually add some information: if the source is known to be on the ground, only the ground value of the retro-plumes is the adjoint; if the source is known to be stationary, the mean value (in time) of the retro-plumes is the adjoint.

From these adjoint functions, a visibility function is computed (Turbelin et al, 2014). The estimated source is then a linear combination of the ratios of the adjoint functions over the visibility function. To optimize the choice of visibility function $\varphi(x)$, the entropy lost (or information gained) by the action of measuring is maximized. The optimal visibility function obeys the following equation:

$$\varphi^2(x) = a^t(x)H_\varphi^{-1}a(x), H_\varphi(x) = \int \frac{a(z)a^t(z)}{\varphi(z)} dz,$$

where $a(x)$ is the adjoint function. Amongst the properties of the visibility function, an important one is that when the real source is a single point source, then the estimated source is maximal at the point of the real source. This allows identifying point releases in the presence of detection and model errors (Issartel et al, 2012). To estimate the intensity of the source q and its position (x,y) , assuming that the source is a point source in the ground plane, that is the source $s(x, y, z) \equiv s_0(x, y) = q_0\delta(x - x_0)\delta(y - y_0)$ is a point source at (x_0, y_0) of intensity q_0 , we minimize the distance between the given measurements μ and the model predicted “measurements” $(s(x, y, z), a(x, y, z)) = q_0(a_1(x_0, y_0), \dots, a_n(x_0, y_0))$ in the renormalized norm induced by $H_\varphi(x)$ i.e. we minimize $\|\mu - q_0(a_1(x_0, y_0), \dots, a_n(x_0, y_0))\|_{H_\varphi}$ over q_0, x_0, y_0 . The consequences of minimizing with respect to the renormalized norm is expanded on in (Issartel et al, 2012).

RESULTS ON SYNTHETIC SENSOR DATA

In order to verify that the inverse methods are working and to give us an idea of what to expect in terms of uncertainties for the Bayesian method we begin with studying the case where sensor measurements have been generated synthetically: the same dispersion model has been used (in forward mode) to simulate the concentrations at the sensor locations as been used to generate the adjoint plumes for inverse modelling. This approach eliminates the errors that would be induced by the fact that the model is a simplified description of the physics it is modelling. Two representative results are shown in **Figure 3**. In the figure, apart from the estimated source locations, the location of the sensors and the geometry, a visualisation of the posterior distribution are shown: it is plotted as a highest posterior density region (HPD) where the color scale shows the highest posterior density (HPD) credibility level. For example, a level curve in the yellow region bounds a HPD area containing almost 100% of the posterior probability mass, whereas a level curve in the blue region bounds a HPD area containing nearly 0% of the posterior probability mass. Hence 0% HPD credibility level represents the maximum posterior density, whereas 100% HPD credibility level represents the minimum posterior density.

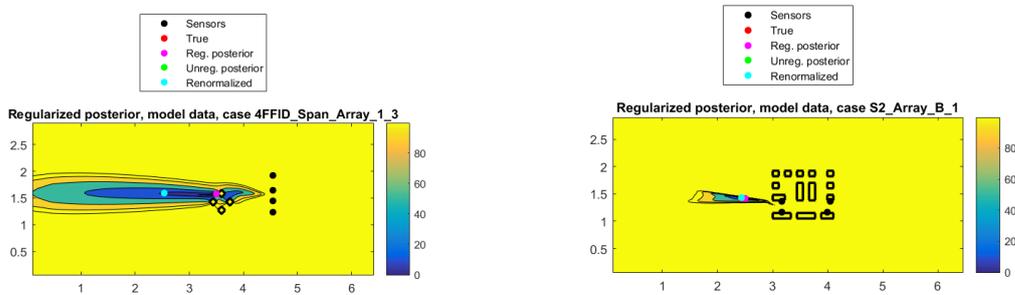


Figure 3 Estimated sources using synthetically generated data. In the left pane the simple array at 45° with sensor configuration B (compare **Figure 1**) is shown, and in the right pane the complex array with sensor configuration B (compare **Figure 2**) is shown. In both panes the estimated source location using Bayes (regularised), pink dot, and the Renormalisation method, cyan dot, are shown as well as the true source location (red dot) – in both panes however the renormalized estimate coincides with the true source location hiding the red dot.

RESULTS ON WIND TUNNEL DATA

Having dealt with the case of synthetically generated measurements we now proceed to the case of estimating the source based on actual measurements in the wind tunnel. We stick to the same cases and configurations as shown in **Figure 3** for easy comparison. See **Figure 4** for the results.

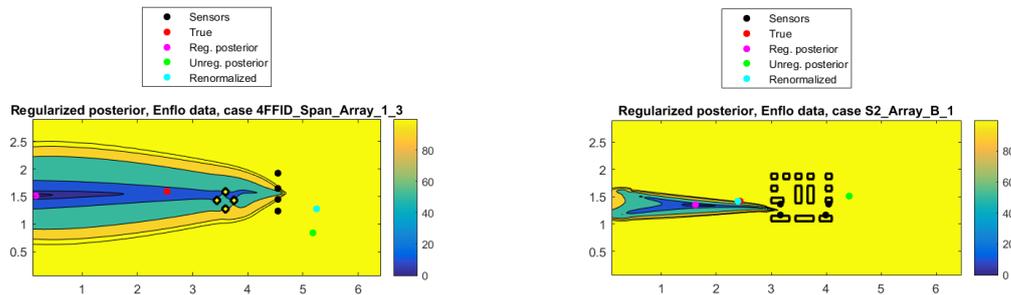


Figure 4 Estimated sources using wind tunnel measurements, same cases as in **Figure 3**. In both panes the estimated source location using Bayes (regularised), pink dot, and the Renormalisation method, cyan dot, are shown as well as the true source location (red dot).

CONCLUSION

Looking at **Figure 3**, where we used synthetically generated data and thus eliminated the error that any model/physics discrepancies would have induced, we conclude that the uncertainties for the Bayesian case are much larger in the wind direction (along the x-axis) compared to the resolution in the cross wind direction (y-direction). Studying the geometry of the visibility function $\varphi(x)$ underpinning the renormalization method we would conclude that the renormalization method suffers from the same feature: the error in source location is larger in the wind direction than in the cross wind direction. We also note that from an inverse modelling point of view the simple array is a harder case. The reason for this is that the source is located relatively far upwind from the buildings, and then the symmetrically positioned buildings scramble the signal that is picked up by a sensor network located far downstream. The Bayesian methods struggles to pinpoint the true source location for wind tunnel measurements as well as synthetic data, even though the true source location is enclosed in the HPD-region with quite high confidence level. The renormalisation method is spot on for synthetic data, but is for some reason disturbed by the wind tunnel measurements. The complex array on the other hand is an easier case, the source is located closer to the buildings (which are not quite symmetric) and the sensors are located within the town. For this complex array case the renormalisation method works beautifully, and the Bayesian method is not far off. Overall we note that when the sensor network has good visibility (in terms of the visibility function $\varphi(x)$) the renormalisation method works well.

ACKNOWLEDGEMENTS

This work was conducted within the European Defence Agency (EDA) project B-1097-ESM4-GP “Modelling the dispersion of toxic industrial chemicals in urban environments” (MODITIC).

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