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INVESTIGATION OF DIFFERENT METHODOLOGIES TO CHARACTERIZE AND PROPAGATE UNCERTAINTIES IN ATMOSPHERIC DISPERSION MODELLING: APPLICATION TO LONG-TERM IMPACT ASSESSMENT

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Abstract: The concentration of a pollutant in the atmosphere is a random variable that can not be modelled deterministically with certainty. Therefore there is a growing demand from regulatory institutions to provide uncertainties regarding the results of environmental impact assessment studies. This paper discusses a probabilistic framework to estimate the impact of various sources of uncertainties on simulation outputs used for environmental impact assessment studies. Using the common framework designed for the treatment of uncertainties in industrial practice, a complete chain for the quantification of uncertainties for environmental impact assessment studies has been developed. A description of each step of the method developed will be given as well as the preliminary results focusing on the uncertainties related to ground-level concentrations.

Key words: *Gaussian plume models, quantification of uncertainties, probabilistic modelling, environmental impact assessment.*

1. INTRODUCTION

Gaussian plume models are commonly used to realize environmental impact assessment (EIA) studies or to evaluate the potential risk associated with accidental release of pollutants in the atmosphere. Despite continuous improvements in atmospheric dispersion modelling, such models are characterized by several sources of uncertainties, in particular:

- In the model inputs: the collection of input data may be inaccurate (emissions, dispersion site characteristics, location of receptors) and the meteorological fields (either derived from measurements or numerical weather prediction models) are uncertain.
- In the physical parameterizations: the parameterizations developed to account for particular physical processes may be viewed as approximations of the reality and then additional sources of uncertainties for numerical modelling.

In the last two decades, several studies tried to address the problem of uncertainties in air quality modelling. In particular, these previous works dealt with the identification of various sources of uncertainties and on the sensitivity and uncertainty analysis methods developed to quantify and/or reduce them (e.g. Hanna *et al*., 1998; Hill *et al*., 2002; Auld *et al*., 2003; Demaël, 2007). For example, using a Computational Fluid Dynamics model, Demaël (2007) has shown that the inverse of the Monin-Obukhov length and the height of the pollutant release were uncertain parameters which strongly impacted ground concentration predictions. A few other studies tried to apply probabilistic method (like ensemble prediction) to air quality forecasting by taking into account several sources of uncertainties associated with input data and physical parameterizations (e.g. Dabberdt and Miller 2000 ; Mallet and Sportisse, 2008). To our knowledge, a few studies tried to transpose probabilistic approaches to EAI studies, in particular considering the whole sources of uncertainties associated with atmospheric dispersion modelling. Actually, the majority of these previous works were mostly focused on a few sources uncertainties and on specific case-studies only considering a few meteorological conditions and thus were not (in theory) applicable to long term studies such as EIA ones.

In the present work, we went further on practical application, focusing on EIA studies at local scale using a Gaussian plume model. We proceeded as follows:

- Identifying and accurately characterizing all sources of uncertainties by assigning probability density functions to uncertain variables (meteorology, emission, grid location, etc.). This may be done using datasets, bibliography or even expert judgment (when no specific information is available).
- Comparing two approaches to quantify uncertainties related to input parameters: a direct one (propagation of uncertainties at each time step) and an indirect one (construction of a probabilistic annual model accounting for uncertainties of meteorological variables).
- Quantifying the effect of input variables uncertainties on simulation outputs (annual mean or hourly percentiles) by performing Monte-Carlo simulations.

We considered a Gaussian plume dispersion model as it is common in EIA. As this kind of model may use various parameterizations of the atmospheric stability (Pasquill-Gifford classes, Doury classes and similitude theory), the impact of input uncertainties has been assessed for each of them.

The paper is structured as follows. In section 2, a description of the approach which has been developed is given. In particular, each step of the chain of quantification of uncertainties associated with ground level concentration prediction will be briefly described. Section 3 presents the first results which have been obtained focusing on the impact of input uncertainties on ground-level concentrations prediction. Some conclusions and perspectives will be drawn in the section 4.

2. DESCRIPTION OF THE CHAIN FOR THE QUANTIFICATION OF UNCERTAINTIES

Following the previous study of Brocheton *et al*. (2008), a chain for the quantification of uncertainties associated with simulation outputs has been developed in accordance with the conceptual scheme for treatment of uncertainties in industrial practice defined by de Rocquigny *et al*. (2008). The approach which has been developed is displayed in Figure 1.

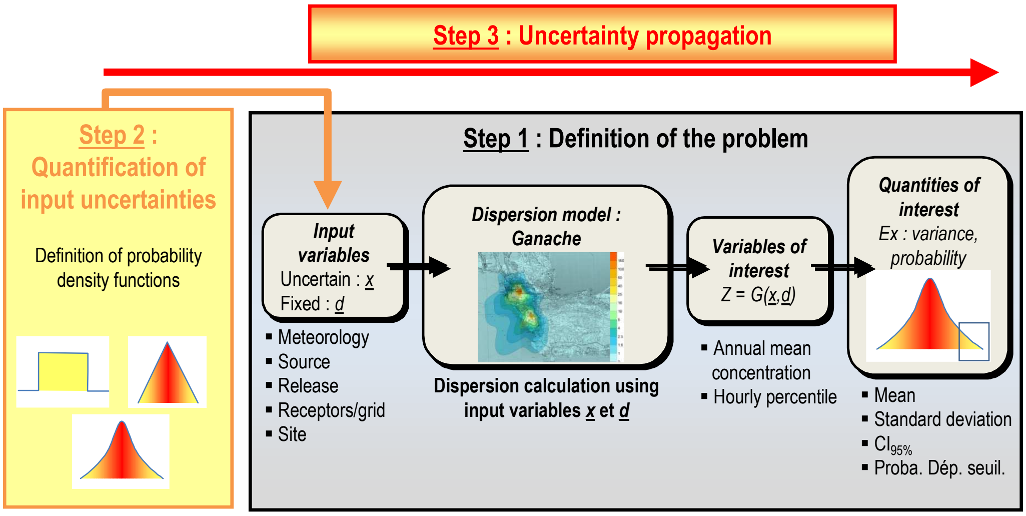

Figure 1. Schematic diagram representing the approach used for the quantification of uncertainties associated with ground-level concentrations (adapted from de Rocquigny *et al*. (2008)).

It is proposed here to briefly describe each step of the approach presented in Figure 1. A thorough review of uncertainty analysis in atmospheric dispersion modelling can be found in Shankar Rao (2005).

2.1 Step 1: Definition of the problem

The first step of our uncertainty analysis consisted of precisely defining the framework of the study, that is: the goal of the uncertainty study, the appropriate case-study, the dispersion model to be used, the input variables, the variables and statistical quantities of interest.

Case-study

The case under study considered a unique source of pollutant of 50 m height with a diameter of 1 m. The source is located at the centre of a domain composed of 50 x 50 points using a horizontal resolution of 100 m. It was hypothesised that the release occurred in flat terrain (considering a uniform rugosity) and that the pollutant was an inert gas. These simplifications implied neglecting uncertainties associated with topography, obstacles, source geometry, physical and chemical transformations of pollutants.

Input variables and variables of interest

As the approach wanted to be exhaustive, it was decided to consider uncertainties related to most of the variables used as input for the dispersion model which was used. In particular, these are the variables defining the meteorology, the dispersion site, the receptors and grid height as well as the characteristics of the release. Note that for meteorology only, a dataset covering five years was used. It comprised wind speed and direction, temperature, cloud cover and precipitation. The other variables related to meteorology were derived from this dataset using the meteorological pre-processor of ADMS (Carruthers, 1994). Stability classes (Pasquill-Gifford and Doury) were computed using the cloud cover and wind speed data.

The annual mean and the 100th hourly percentile of the ground-level concentration have been chosen as variables of interest as these are variables that may be used in typical EIA studies.

Dispersion model

The Gaussian plume model GANACHE has been chosen to conduct the numerical experiments. This model is currently developed at Central School of Lyon (France) and may use various parameterizations of atmospheric stability, that is similitude theory, Pasquill-Gifford and Doury classes. Although each type of parameterization has been used for numerical applications, in the present paper, we will only focus on numerical experiments using similitude theory.

Quantities of interest and goal of the study

The main goal of the study was to quantify the impact of input uncertainties on ground-level concentration simulations in the framework of EIA studies. It was decided to adopt a probabilistic approach to estimate the dispersion of the results, using mean values and standard deviation of the distribution of the variables of interest.

2.2 Step2: Quantification of input uncertainties

This step consisted of assigning probability distribution function to each input variable considered as uncertain (probability density function (PDF) or cumulative density function (CDF)). For a given variable, there are three ways to define its probability distribution. When measurements of this variable are available, it is possible to define its PDF directly using these data. When no data are available, it is possible to define the PDF of the variable using either results from past studies (bibliography) or expert judgment.

In the present study, two methods were carried out to derive and propagate PDF associated with input variables related to meteorology:

- The so-called *direct method* which consisted of adding uncertainties to each meteorological variable for every time step. At each time step, the value of a given variable equals its deterministic value plus a measure of its uncertainty. Actually, the uncertainty added at each time step may be viewed as a probable value of the error of measurement associated with the variable which is considered.
- The so-called in*direct method* which consisted of generating a probabilistic model from statistical analysis of input data. For each meteorological variable, it consisted of finding the PDF the best fitting its real distribution. After having defined each PDF, the second step was to define linear and rank correlations between input variables to account for possible dependencies when building the probabilistic model. If these dependencies are implicitly taken into account using the direct approach, it needs to be precisely defined when using the indirect one.

The PDF of input variables related to the characteristics of the release, the dispersion site, and receptors and grid heights were mainly defined from expert judgment and did not vary between direct and indirect methods. The PDF used for input variables for each of the direct and indirect methods are given in Table 1.

Table 2. Definition of the probability density functions used for uncertain input variables.

Variable	Direct approach	Indirect approach
Wind speed ($m.s^{-1}$)	Normal (mean = 0; sigma = 0.15[1])	Weibull (α = 3.6026; β = 1.5086; γ = 0)
Wind direction (°)	Normal (mean = 0; sigma = 13.7[1])	Truncated mixture of normal laws
Temperature (°C)	Not used	Normal (mean = 12.19; sigma = 7.76)
Cloud cover (oktas)	Normal (mean = 0; sigma = 1)	Not used
Boundary layer height (m)	Normal (mean = 0; sigma = 25)	Weibull (α = 343.15; β = 0.92; γ = 0)
Inverse of the Monin-Obukhov length (m)	Derived from other input variables	Kernel Smoothing fitting
Dispersion site rugosity (m)	Uniform (min = 0.4; max = 0.7)	Uniform (min = 0.4; max = 0.7)
Temperature of the pollutant release	Normal (mean = 50; sigma = 1)	Normal (mean = 50; sigma = 1)
Speed of the pollutant release ($m.s^{-1}$)	Normal (mean = 12; sigma = 1)	Normal (mean = 12; sigma = 1)
Quantity of pollutant released ($g.s^{-1}$)	Uniform (min = 7; max = 13)	Uniform (min = 7; max = 13)
Grid and receptors height (m)	Triangular (min = 1; max = 2; mode = 1.5)	Triangular (min = 1; max = 2; mode = 1.5)

2.3 Step3: Uncertainty propagation

This step of the uncertainty analysis consisted of propagating the joint PDF of each input variable through the dispersion model to generate the PDF of the model results, that is, of the variables of interest. Considering it is the reference method for probabilistic modelling, Monte Carlo simulations were used to propagate input uncertainties. Such a method involves random sampling from the PDF of each input variable and successive models run until obtaining a statistical distribution of each variable of interest. Monte Carlo methods have already been applied to atmospheric models ranging from simple Gaussian plume models (Kocher *et al*., 1987; Irwin *et al*., 1987) to complex Computational Fluid Dynamics models (Demaël, 2007).

The period for uncertainty propagation has been reduced from five years to one year only considering the computational cost associated when using the five year period. Using the so-called direct method, 100 Monte Carlo runs were conducted per time-step for the whole year of study. This represented 876,000 integrations of the dispersion model and approximately 5 days of computations. The indirect method differed from the direct one as it did not account for the temporal dimension. Uncertainty propagation is then performed using a restricted number of Monte Carlo runs. Here, an arbitrary number of 8000 runs was used. Note that for the present study, we did not consider possible dependencies between input variables when using the indirect approach.

3. PRELIMINARY RESULTS

In this section, we will only focus on results regarding ground-level concentrations simulations.

[1] Arithmetic means based on the work of Hill *et al*. (2002).

3.1 Comparisons between deterministic and probabilistic modelling

The Figure displays the mean annual concentration and the 100th hourly percentile derived from deterministic and probabilistic runs that used the direct approach described in sections 2.2 and 2.3.

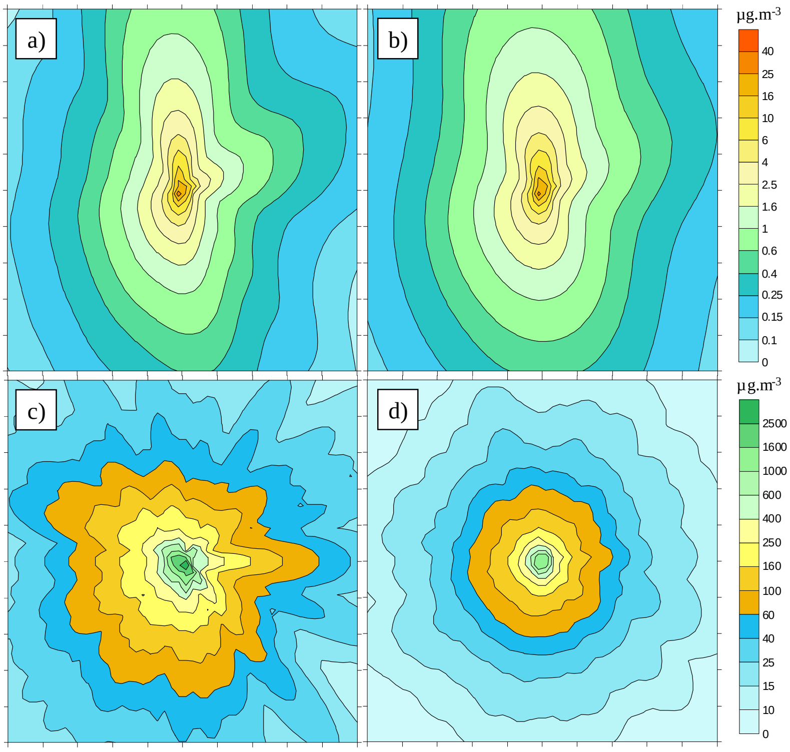

Figure 2. Mean annual concentration (µg.m^{-3}) derived from (a) the deterministic run and (b) the direct probabilistic approach. (c) and (d) as (a) and (b) but for the 100th hourly percentile of the predicted concentrations (µg.m^{-3}).

Apparently, the results derived from probabilistic simulations are smoothed in comparison with deterministic ones. In terms of annual mean concentrations, the probabilistic approach differed from the deterministic one by more or less 3 µg.m^{-3} in the vicinity of the release (at a distance of approximately 250 m) that is, almost 10% of the deterministic value. The impact of input uncertainties on the numerical prediction of ground-level concentrations is much more striking when looking at the results concerning the 100th hourly percentile. In particular, the deterministic run produced higher values than the probabilistic approach over the whole simulation domain (differences reaching more than 2000 µg.m^{-3} and 250 µg.m^{-3} at 250 m and 1000 m of the release, respectively). Note that the dispersion (i.e. the standard deviation of the ensemble results) of the variables of interest remained very small (less that 1% of the ensemble mean) even at very short range of the release (not shown).

3.2 Comparisons between the direct and indirect probabilistic approaches

The comparison of the so-called direct and indirect methods has been achieved performing numerical calculations considering fixed receptors only. The receptors have been placed according to two particular wind directions identified from the dataset which has been used: one rather infrequent (direction D1) and the other frequently observed (direction D2). For each direction, four receptors have been placed at various distances of the release: 250, 500, 1000 and 2000 m. The results obtained with the direct and indirect approaches are shown on Figure 3.

The mean annual concentrations predicted by the two methods (direct and indirect, Figurea) are larger in direction D2 and tend to decrease when the distance from the release increases. Moreover, we can note that the direct approach simulates larger concentration values than the indirect one, especially in the vicinity of the release. The differences between the two approaches become negligible for the receptors located at 500 m or more from the source. The simulated 100th percentiles exhibit more discrepancies between the two methods as the indirect one tends to strongly overestimate the simulated concentrations derived from the direct approach (Figureb). Actually, the 100th percentiles derived from the indirect approach ranges between 2 to 4.5 times the results provided by the direct method.

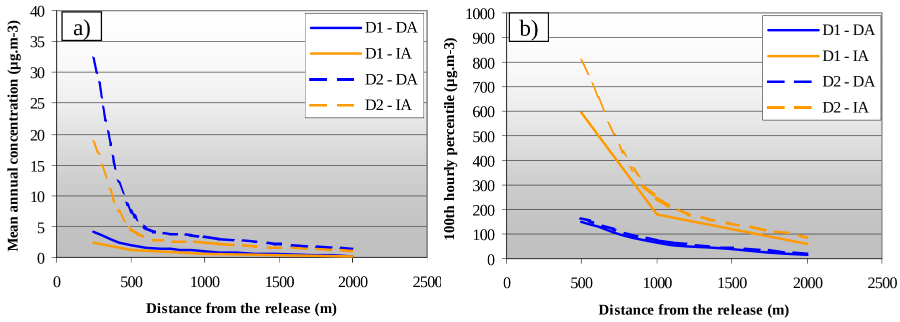

Figure 3. (a) Mean annual concentration and (b) 100th hourly percentile ($\mu g.m^{-3}$) as a function of the distance from the release. *D1* (resp. *D2*) is used for the wind direction frequently (resp. rarely) observed and *DA* (resp. *IA*) for the direct (resp. indirect) approach.

3.3 Uncertainty related to the location of receptors

The definition of the location of receptors is prone to high uncertainties. For example, when defining a hospital as a particular receptor, one will choose the centre of the hospital to define the receptor location while this hospital can not be simply reduced to a single point. To have an idea of the uncertainty related to such a method to define the location of receptors, we reproduced the experiment described in section 3.2 using the direct approach only. Moreover, for each receptor located both in the D1 and D2 directions, we defined four points surrounding it at a distance of more or less 50 m. Doing this for each receptor, we computed the normalised standard deviation of the mean annual concentration and the 100th percentile between this receptor and the four surrounding ones. The results showed that the normalised standard deviation of each variable of interest ranged around 50% of the mean value in the vicinity of the release, suggesting a high variability of the results and thus a strong uncertainty related to the location of the receptors.

4. CONCLUSIONS AND FUTURE WORK

In this study, a chain for the quantification of the impact of input uncertainties on ground-level concentrations simulations has been developed. The experiments which have been conducted suggested that considering uncertainties related to input data may involve different results than those provided by simple deterministic approaches. At this point of the study, it has not been possible to show which one of the direct and the indirect approach was more appropriate for probabilistic modelling applied to long term impact assessment studies. Finally, the high uncertainty related to the definition of single receptors for specific establishments (schools, hospitals, etc.) has also been pointed out. It is planed to follow through this study mainly focusing on the implementation of alternative uncertainty propagation methods (for example polynomial chaos expansion), the representation of dependencies between input variables when using the indirect approach and on the realization of sensitivity analyses (that is ranking uncertainty sources as a function of their importance regarding the simulation results).

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