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Sensitivity analysis of a model for atmospheric dispersion of toxic gases

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Abstract

We study the relative influence of uncertainty in input parameters of an atmospheric dispersion model on the variation of the outputs. Sensitivity indices are calculated using the FAST and Sobol' methods on a passive gas dispersion scenario, using the PHAST tool. We assess both the individual and coupled influence of parameters.

Keywords: Industrial risk, Sensitivity analysis, Gas dispersion modelling

1. Introduction

Recent changes to French legislation concerning the prevention of technological and natural risks require industrial sites to calculate the safety perimeters for different accident scenarios, based on a detailed probabilistic risk assessment. It is important that safety perimeters be based on the best scientific knowledge available, and that the level of uncertainty be minimised. A significant contribution to the calculation of the safety zones comes from the modelling of atmospheric dispersion, particularly of the accidental release of toxic products.

One of the most widely used tools for dispersion modelling in several European countries is PHAST™ (DNV Software, UK). This software application is quite flexible, allowing the user to customize values for a wide range of model parameters. Users of the software have found that simulation results may depend quite strongly on the values chosen for some of these parameters. While this flexibility is useful, it can lead different users to calculate effect distances that vary considerably even when studying the same scenario (CCPS, 1996).

Sensitivity analysis techniques can be used to measure the effect on the variation in the model output due to variation in input parameters. Several sensitivity analysis (SA) methods exist, including one-at-a-time (OAT) method, fractional experiments, differential analysis, Fourier Amplitude Sensitivity Test (FAST) and Sobol'. Several sensitivity analysis of various dispersion software tools have been carried out using OAT method (Bubbico and Mazzarotta, 2007; DNV, 2006; Nair et al., 1997).

The objective of this study is to carry out a sensitivity analysis of PHAST dispersion modelling using global methods such as FAST and Sobol'. We have developed a methodology and applied it to a case study of a gas passive dispersion scenario.

2. Software tools

2.1. PHAST

PHAST (Process Hazard Analysis Software Tool) is a comprehensive consequence analysis tool. It examines the process of a potential incident from the initial release to far field dispersion, including modelling of pool vaporisation and evaporation, and flammable and toxic effects. PHAST is able to simulate various release scenarios such as leaks, line ruptures, long pipeline releases and tank roof collapse in pressurised / un-pressurised vessels or pipes. These source terms are combined with the PHAST dispersion model called UDM (Unified Dispersion Model) (DNV, 2005) to obtain desired consequence results: i) cloud behaviour ii) transition through various stages such as jet phase, heavy phase, transition phase and passive dispersion phase, iii) distance to hazardous concentration of interest and iv) footprint of the cloud at a given time.

PHAST release and dispersion models are also available in the form of an Excel interface, called MDE Generic Spreadsheets™. Sensitivity studies can be easily carried out using these Spreadsheets, since they allow direct control of input parameters and output results, easy parameter variation and multiple runs (simultaneous simulation of various scenarios). PHAST v.6.53 has been used in this work.

2.2. SimLab

SimLab (Simulation Laboratory for Uncertainty and Sensitivity Analysis) is a software tool (JRC, Italy, 2006) designed for Monte Carlo (MC) analysis that is based on performing multiple model evaluations with probabilistically selected model input. The results of these evaluations are used to determine 1) the uncertainty in model predictions and 2) the input variables that give rise to this uncertainty.

SimLab generates a sample of points based on the range and distribution of each input parameter specified by the user. For each element of the sample, a set of model outputs is produced by evaluating an internal or external model. In essence, these model evaluations create a mapping from the space of the inputs to the space of the results. This mapping is the basis for subsequent uncertainty and sensitivity analysis to calculate various sensitivity indices.

3. Sensitivity analysis (SA)

SA is the study of how the variation in the output of a model can be apportioned, quantitatively or qualitatively, to variation in the model parameters (Saltelli et al., 2004). Saltelli (2004) proposes one possible way of grouping these methods into three classes: screening methods, local SA methods and global SA methods.

3.1. Screening methods

SA is the study of how the variation in the output of a model can be apportioned, quantitatively or qualitatively, to variation in the model parameters (Saltelli et al., 2004). Saltelli (2004) proposes one possible way of grouping these methods into three classes: screening methods, local SA methods and global SA methods.

3.2. Local SA methods

They are useful for models which are computationally expensive to evaluate and/or have a large number of input parameters. Various strategies and methods have been discussed in several articles with illustrative examples: Bettonvil and Kleijnen, 1997; Campolongo and Braddock, 1999; Deana and Lewis, 2002; Morris, 2006.

3.3. Global SA methods

Global SA techniques incorporate the whole range of variation and the probability density function of the input parameters to calculate their influence on the output. Many global sensitivity analysis techniques are now available, such as Fourier Amplitude Sensitivity Test (FAST) (Saltelli et al., 2005; Xu and Gertner, 2007a), regression-based methods (Helton et al., 2005) and Sobol's method (Sobol', 1993). A survey of sampling-based methods has been presented by Helton et al. (2006). Most of the global methods, such as FAST and Sobol' rely on the assumption of parameter independence (Xu and Gertner, 2007b).

The quantitative measure of sensitivity is represented by *Sensitivity Indices*. The first-order sensitivity index, S_i of an input factor p_i is the measure of the main (direct) effect of p_i on the output variance. S_{ij} (where $i \neq j$), the second-order sensitivity indices, measures the interaction effect of p_i and p_j on the output variance. Other higher-order indices are defined in the same manner. The total sensitivity index, S_{Ti} is the sum of all sensitivity indices involving factor p_i (Homma and Saltelli, 1996). For example, the total sensitivity index of factor 1, S_{T1} for a model with 3 input factors is given as:

$$S_{T1} = S_1 + S_{12} + S_{13} + S_{123}$$

Total indices are especially suited to apportion the model output variation to the input factors in a comprehensive manner. The FAST method calculates the first-order and total sensitivity indices, whereas Sobol' method, in addition to these, also provides all higher-order sensitivity indices to determine quantitatively the interaction between parameters. But with Sobol', as number of indices to be calculated is very high, computational cost and calculation time go high.

The first-order (S_i) and total (S_{Ti}) indices can be interpreted as following:

- S_{Ti} high: p_i is an influent parameter
- S_i and S_{Ti} both small: p_i is not an influent parameter (neither alone nor in interaction with other parameters)
- S_i and S_{Ti} nearly the same: no interaction of p_i with other parameter
- S_i and S_{Ti} very different: high interaction of p_i with other parameter

4. Methodology

We have developed a method to carry out sensitivity studies by linking PHAST Spreadsheet and SimLab. Our method comprises of six steps, as shown in the Fig. 1.

❶: The description of input parameters defined by the user is sent to SimLab.

❷: The set of sample element created by SimLab is saved in the controller.

❸ and ❹: For each element of the sample, PHAST calculates the output, which is sent to the controller.

❺ The set of PHAST outputs is transferred to SimLab.

❻ Depending on the selected sensitivity analysis method (FAST or Sobol'), SimLab calculates various sensitivity indices (1^{st} order, 2^{nd} order, …, Total order).

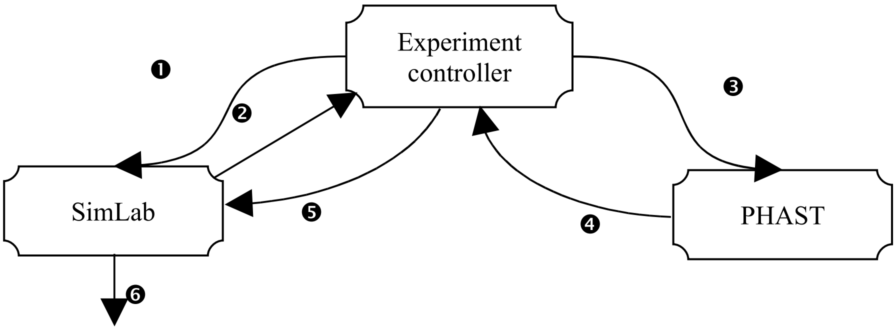

Figure 1: Methodology for sensitivity analysis

5. Case Study

We have studied a scenario of passive dispersion of air (as a pollutant) in the atmosphere. The base case is defined as a continuous release in the following conditions: duration of 360 000 s, release rate 0.05 kg/s, release height 50 m, temperature 298 K and release velocity 5 m/s. The ambient conditions are: Pasquill stability class D, wind speed 5 m/s, temperature 298 K, solar flux 500 W/m^2, molecular weight 28.966, logarithmic temperature and linear pressure profiles. Dispersion is considered over land: dry soil, temperature 298 K and surface roughness of 0.1 m. Averaging time is set to 600 s. This case study can be calculated analytically by TNO passive dispersion equation (Dujim et al., 1996).

In order to choose the relevant model outputs, the concentration profile of pollutant at the ground level as a function of the downwind distance from the release point is calculated with PHAST for the base case as shown in Figure 2.

The following model outputs are considered for the analysis:

Output 1. Ground level concentration at 200 m downwind distance
Output 2. Ground level concentration at 10 000 m downwind distance
Output 3. Maximum downwind distance at the ground level concentration of 0.1 ppm
Output 4. Downwind distance at which highest ground level concentration is observed
Output 5. Maximum crosswind distance at the ground level concentration of 0.1 ppm

Fig. 2 shows relative good agreement between analytical and PHAST results.

The description of the independent input parameters is given in Table 1. The values of remaining parameters are kept constant as defined in the base case.

Table 1: Input Parameters

	Parameters	Type of distribution	Parameter range		Unit
			Min	Max	
Z0	Height of release	Continuous uniform	0	700	m
Q	Release rate	Continuous uniform	0.005	50	kg/s
ua	Wind speed	Continuous uniform	1	11	m/s
tav	Averaging time	Continuous uniform	18.75	3600	s

ZR	Surface roughness	Discrete uniform	0.0001; 0.001; 0.01; 0.1; 1; 3	m

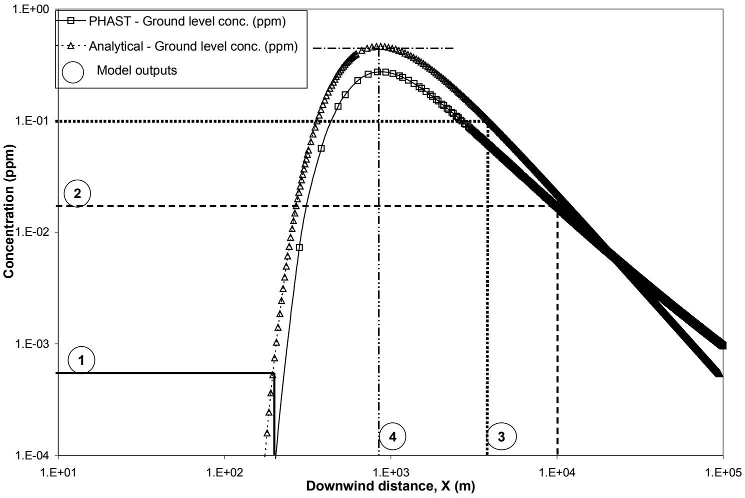

Figure 2: Ground level concentration vs. downwind distance for the base case

6. Results and discussion

For each output, the objective of the FAST global analysis is to determine which parameters are influent/non-influent, to appreciate the relative influence of parameters and to assess qualitatively interaction between parameters. Table 2 shows the results of FAST method with sample size of 100 000 points.

Table 2: FAST sensitivity analysis results

	z0		tav		zr		Q		ua	
	S_i	S_{Ti}	S_i	S_{Ti}	S_i	S_{Ti}	S_i	S_{Ti}	S_i	S_{Ti}
Output 1	0.054	0.881	0.001	0.097	0	0.182	0.003	0.277	0.006	0.367
Output 2	0.276	0.658	0.161	0.103	0	0.098	0.105	0.351	0.173	0.496
Output 3	0.005	0.226	0.009	0.304	0.004	0.305	0.283	0.879	0.067	0.617
Output 4	0.772	0.835	0	0.006	0.163	0.229	0	0.006	0	0.007
Output 5	0.031	0.595	0.001	0.282	0.002	0.331	0.285	0.899	0.009	0.496

The interpretation of the above results is summarised in Table 3.

Table 3: Interpretation of FAST sensitivity analysis results

Outputs	Influent parameters in decreasing order	Interaction between parameters
Output1	Z0, Q, ua	Z0, Q, ua
Output2	Z0, Q, ua	Z0, Q, ua
Output3	Q, ua	Q, Z0, ua
Output4	Z0	-
Output5	Q, Zr	Q, Z0, ua

Sobol' method is used to determine quantitatively the interaction between parameters. As an example, Fig. 3 shows a pie chart of all higher-order sensitivity indices relative to Z0 for the output C at 200m.

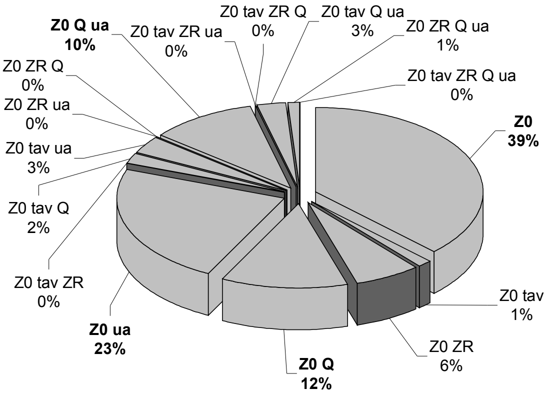

Figure 3: Sensitivity analysis results of SOBOL' for model output C at 200m and related to input factor Release height, Z0

Fig. 3 shows that 85 percentage of total sensitivity index of release height is composed of 39% main effect of Z0, 23% interaction effect between Z0 and ua, 12 % interaction effect between Z0 and Q and 10% interaction effect of Z0, Q and ua.

The main problems encountered in this work were: i) very long computational time and ii) absence of PHAST output for some of the sample elements (for output3 and output5).

7. Conclusion

We have developed a method to carry out sensitivity analysis of PHAST dispersion model and applied it to a passive gas dispersion scenario. In further work, we shall apply it to more complex dispersion scenarios. However, the treatment of dependent input parameters shall require modification in the sampling procedure.

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