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# Toxic Release Dispersion Modelling with PHAST: Parametric Sensitivity Analysis

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The objective of this study is to carry out a parametric sensitivity analysis of PHAST atmospheric dispersion modelling for an accidental toxic gas release scenario. A methodology is developed and is applied to a nitric oxide gas dispersion scenario. We study the relative influence of uncertainty in independent input parameters (storage conditions, atmospheric variables, release parameters and orographic conditions) on the variation of the model outputs (concentrations in the near and far fields, distance at which maximum concentration is observed and downwind distance where cloud dispersion profile becomes passive). The Fourier Amplitude Sensitivity Test (FAST), a global sensitivity analysis method, is chosen to calculate first-order and total sensitivity indices. These indices provide a measure of both the individual effects and coupled influence of parameters.

## 1. Introduction

An accidental toxic gas release may have serious consequences on neighbouring population. Concern for public safety has led to the establishment of safety perimeters, within which land use planning is strictly controlled. It is important that these safety perimeters be established using 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<sup>TM</sup> (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 considerably on the values chosen for some of these parameters. While this flexibility is useful, it can lead to disparities in the calculations of effect distances even when studying the same scenario. Sensitivity Analysis (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 input parameters (Saltelli et al., 2004). Several sensitivity analysis methods exist, such as one-at-a-time (OAT) methods, Fourier Amplitude Sensitivity Test (FAST) and Sobol'.

In literature related to atmospheric dispersion modeling, there are essentially sensitivity analysis studies based on OAT method. For example, Bubbico and Mazzarotta (2007) have applied an OAT method to a 15-minute accidental toxic release scenario. The parameters studied are Pasquill stability class, wind speed, ambient temperature and release hole diameter. In this study, ALOHA (EPA, USA) and Trace 9.0 (Safer systems, USA) software tools have been used to calculate distances corresponding to ERPG-2 and IDLH of hydrogen chloride, ammonia, trimethylamine and bromine. Moreover, the

Unified Dispersion Model (UDM) verification manual (DNV, 2006) describes a sensitivity analysis of PHAST. An OAT method has been employed for various release scenarios, studying parameters such as release height, release velocity, surface roughness, and stability class.

The objective of this study is to carry out a sensitivity analysis of PHAST dispersion modelling for toxic gas release scenarios using FAST global SA method. For this purpose, a methodology is developed and is illustrated through a nitric oxide gas dispersion scenario. The main input parameters involved in the calculation of various model outputs are related to storage, atmospheric, release and orographic conditions. The effect of their variability, within specific intervals and according to their distribution type, on the results has been evaluated.

## **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 / unpressurised vessels or pipes. An integral-type dispersion model called UDM (Unified Dispersion Model) calculates several 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 *i*) the uncertainty in model predictions and *ii*) 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)

The aim of SA is to determine: *i*) the factors that contribute the most to the output variability, *ii*) the model parameters that are negligible (since they have little impact on the outputs), *iii*) interaction effects of parameters.

Saltelli et al. (2004) proposes one possible way of grouping these methods into three classes: screening methods, local SA methods and global SA methods.

**Screening methods.** The aim of screening methods is to identify the most important parameters from amongst a large number that affect model outputs. 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: Campolongo et al., 2007; Morris, 2006.

**Local SA methods.** Local SA methods provide the slope of the calculated model output at a given point in the input space (Turányi and Rabitz, 2004). However, local sensitivity analysis can only inspect one point at a time and the sensitivity index of a specific parameter depends on the central values of the other parameters. Thus, more studies are currently using global SA methods instead of local SA ones (Xu and Gertner, 2007a).

**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 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 a 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  $p_1$ ,  $S_{T1}$  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's method, in addition to these, also provides all higher-order sensitivity indices to determine quantitatively the interaction between parameters. However, the computational cost implied by Sobol's method increases significantly as the number of indices to be calculated is increases.

### 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 Figure 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.

- ⑤ The set of PHAST outputs is transferred to SimLab.
- ⑥ Depending on the selected sensitivity analysis method (FAST or Sobol'), SimLab calculates various sensitivity indices (1<sup>st</sup> order, 2<sup>nd</sup> order, ..., Total order).

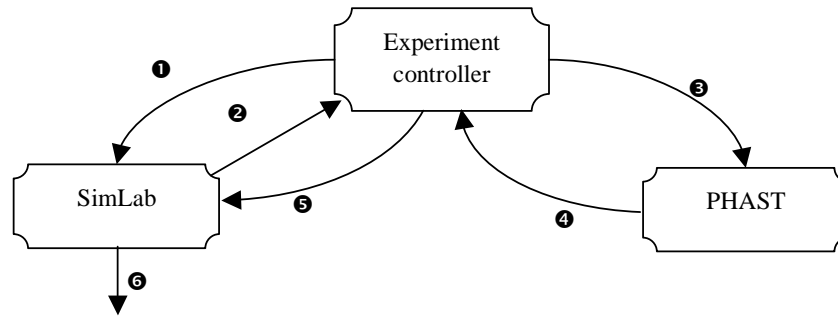


Figure 1: Methodology for sensitivity analysis

## 5. Case Study

We have studied a nitric oxide gas release scenario. Nitric oxide (NO) is stored in a pressurized tank and it is assumed that there is sufficient quantity of NO available for continuous discharge up to 3600 seconds. The source term considered is “Leak”: a hole in the tank results in the release of NO to the atmosphere. The discharge calculations are carried out in PHAST using “Orifice” model, which calculates release rate and state of the gas after its expansion to the atmospheric pressure.

These discharge data are used by UDM for the consequence calculations. UDM simulates the progression of the cloud through several phases: jet, heavy, transition and passive (Gaussian concentration profile) phase. As NO is not a heavy gas, only three phases have been observed during the dispersion of its cloud: jet phase, transition phase and passive phase. The jet phase is dominant initially, followed by the transition phase and the full passive phase. Each phase uses a separate set of correlations to calculate the dimension and concentration of the cloud in the downwind direction. The starting of the transition phase depends on several criteria, such as maximum difference between cloud and wind speeds and maximum difference between cloud and atmosphere densities. This transition is needed to avoid discontinuous entrainments and spread rates.

The scenario is defined as follows: continuous horizontal release over land, Pasquill stability class D, temperature of dispersing surface equals to atmospheric temperature. The following model outputs are considered for the analysis:

- Output 1. Concentration at 200 m downwind and at 1.5 m height (C200)
- Output 2. Concentration at 1 000 m downwind and at 1.5 m height (C1k)
- Output 3. Concentration at 10 000 m downwind and at 1.5 m height (C10k)
- Output 4. Downwind distance and at 1.5 m height, where highest concentration is observed (Xcmax)
- Output 5. Downwind distance where transition to passive phase occurs (Dtr)

The description of the independent input parameters studied is given in Table 1. They concern storage ( $Pst$ ,  $Tst$ ), atmospheric ( $Pa$ ,  $Ta$ ,  $Ha$ ,  $Cpa$ ,  $Ua$ ,  $Wp$ ,  $TPp$ ), release ( $Do$ ,  $Dur$ ,  $ZR$ ) and orographic conditions ( $ZO$ ). Other model parameters are kept at their default values as defined in the PHAST software.

Table 1: Input Parameters

Parameters	Type of distribution	Parameter range		Unit	
		Min	Max		
Pst	Storage pressure	Continuous uniform	$1.20 \cdot 10^5$	$5.00 \cdot 10^6$	Pa
Tst	Storage temperature	Continuous uniform	248.15	323.15	K
Do	Orifice diameter	Continuous uniform	0.001	0.6	m
Pa	Atm. Pressure	Continuous uniform	$10^5$	$1.20 \cdot 10^6$	Pa
Ta	Atm. Temperature	Continuous uniform	223.15	323.15	K
Ha	Atm. Humidity	Continuous uniform	0.3	1	-
Dur	Duration of release	Continuous uniform	18.75	3600	s
ZO	Surface roughness	Continuous uniform	$10^{-10}$	3	M
ZR	Release height	Continuous uniform	0	50	M
Ua	Wind speed	Continuous uniform	1	15	$m \cdot s^{-1}$
Cpa	Atm. Sp. Heat	Continuous uniform	800	1200	$J \cdot kg^{-1} \cdot K^{-1}$
Wp	Wind profile	Discrete uniform	1, 2*	-	-
TPp	T/P profile	Discrete uniform	1, 2, 3**	-	-

\*1 = uniform (constant), 2 = power law

\*\*1 = both uniform (constant), 2 = both linear, 3 = logarithmic temperature and linear pressure

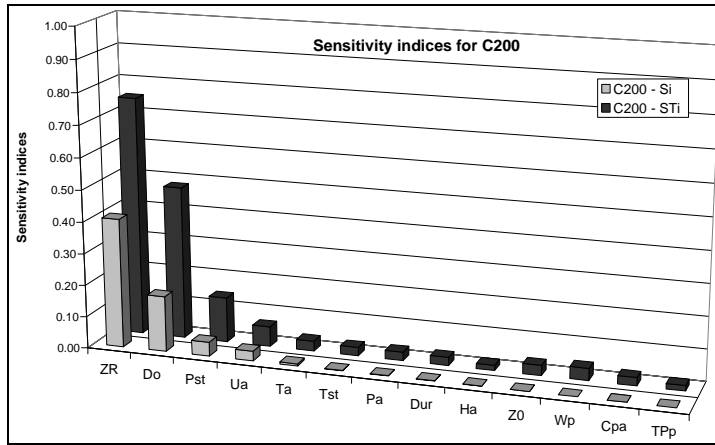
## 6. Results and Discussion

The FAST global SA method has been applied with a sample size of 10 000 points. Figure 2 represents the first-order ( $S_i$ ) and total ( $S_{Ti}$ ) sensitivity indices for the model outputs  $C200$ ,  $C10k$  and  $Xcmax$ .

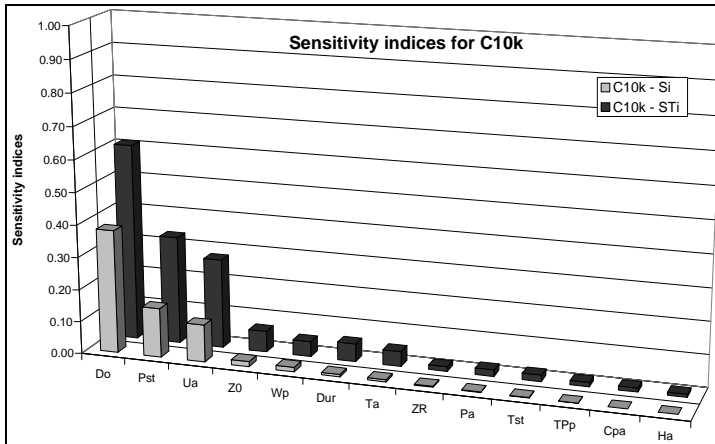
For the output  $C200$  (Figure 2a), it can be observed from the  $S_i$  values that release height ( $ZR$ ) and orifice diameter ( $Do$ ) have a strong impact on this output variance. Furthermore, high  $S_{Ti}$  values of these parameters suggest that there is a strong interaction between these two parameters.

For the model output  $C10k$  (Figure 2b), orifice diameter ( $Do$ ), storage pressure ( $Pst$ ) and wind speed ( $Ua$ ) are the most influential parameters (alone and interaction).

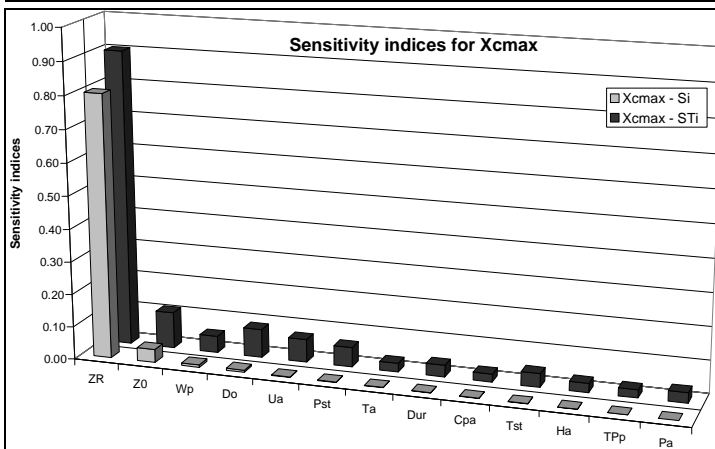
For the model output  $Xcmax$  (Figure 2c), only  $ZR$  is an influent parameter:  $Xcmax$  increases when  $ZR$  increases.



a)



b)


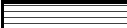


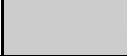


c)

Figure 2: First-order ( $S_i$ ) and total ( $S_{Ti}$ ) sensitivity indices for model outputs: a) Concentration at 200 m, b) Concentration at 10 000 m, c) Downwind distance at maximum concentration

The first-order ( $S_i$ ) and total ( $S_{Ti}$ ) indices for a parameter  $p_i$  can be interpreted as shown in Table 2.


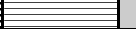
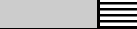


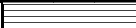
























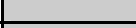
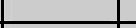
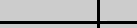


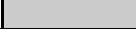
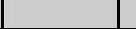
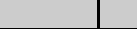












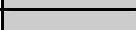
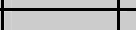
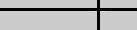


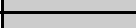
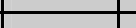
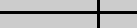







Table 2: Interpretation of sensitivity indices

$S_i$ and $S_{Ti}$	Interpretation	Symbol
$S_i > 0.3$	$p_i$ is a very influent parameter (alone)	
$0.1 < S_i < 0.3$	$p_i$ is an influent parameter (alone)	
$S_i < 0.1$ and $S_{Ti} > 0.3$	$p_i$ is not influent alone but shows strong interactions with other parameters	
$S_i < 0.1$ and $0.1 < S_{Ti} < 0.3$	$p_i$ is not influent alone but shows some interaction with other parameters	
$S_i < 0.1$ and $S_{Ti} < 0.1$	$p_i$ is not an influent parameter (neither alone nor in interaction with other parameters)	

Parametric sensitivity analysis results are shown in Table 3 for all model outputs. This table serves to compare the influence of the various input parameters on the different model outputs.

For outputs  $C200$ ,  $C1k$  and  $C10k$ , it can be observed that  $ZR$  is a very influent parameter in the near-field, but is not influent in the far-field. Moreover, wind speed has influence only on the far-field concentrations.  $Do$  is influent for all three outputs.  $Pst$  has mainly a direct influence on the far-field concentrations.

Table 3: Parametric sensitivity analysis results

Parameters \ Outputs	$C200$	$C1k$	$C10k$	$Xcmax$	$Dtr$
$ZR$					
$Do$					
$Pst$					
$Ua$					
$Ta$					
$Tst$					
$Pa$					
$Dur$					
$Ha$					
$Z0$					
$Wp$					
$Cpa$					
$TPp$					

\*signification of symbols is given in Table 2

The distance to passive transition (Figure 3) is moderately influenced by direct variations in  $Pst$  and  $Ua$ , but it is highly influenced by the combined effect of  $Do$ ,  $Pst$ ,  $Ua$ ,  $Pa$  and  $Z0$ .



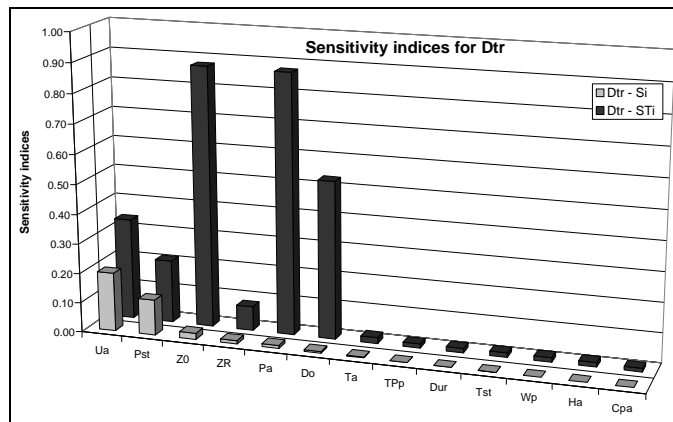


Figure 3: First-order ( $S_i$ ) and total ( $S_{Ti}$ ) sensitivity indices for the model output transition distance to passive phase

## 7. Conclusion

We have developed a methodology to carry out parametric sensitivity analysis (using the FAST method) of the PHAST dispersion model and applied it to an accidental nitric oxide gas dispersion scenario. This study allows the identification of which parameters most influence concentrations in near and far fields, downwind distance where highest concentration is observed and transition distance where cloud behaviour enters passive phase. Combined effects of parameters are evaluated qualitatively. In further work, we shall widen our study to include all parameters, such as internal model parameters, jet model parameters, heat transfer between land and the cloud, and transition to passive phase control parameters. The methodology shall be adapted to allow correlations between input parameters to be taken into account.

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