Sensitivity analysis of atmospheric dispersion modeling in emergency situation

Stéphane Pagnon, Aurélia Bony-Dandrieux, Jérôme Tixier, Gilles Dusserre, Bruno Debray, François Fontaine

HAL Id: ineris-00976229
https://ineris.hal.science/ineris-00976229

Submitted on 9 Apr 2014

Sensitivity Analysis of Atmospheric Dispersion Modeling In Emergency Situation

PAGNON Stéphane
INERIS Parc Technologique ALATA, BP2 60550 Verneuil-en-Halatte, France
stephane.pagnon@ineris.fr

BONY-DANDRIEUX Aurelia, TIXIER Jerome, DUSSERRE Gilles
LGEI, Ecole des Mines d'Alès, 6 avenue de Clavières 30319 Alès, France
Aurelia.Bony-Dandrieux@mines-ales.fr, Jerome.Tixier@mines-ales.fr,
Gilles.Dusserre@mines-ales.fr

DEBRAY B., FONTAINE F.
INERIS Parc Technologique ALATA, BP2 60550 Verneuil-en-Halatte, France
bruno.debray@ineris.fr, francois.fontaine@ineris.fr

Abstract

Each day, accidents involving hazardous materials are managed by Emergency Services. In order to bring the best adapted operational answer, it is necessary to determine with accuracy the concentrations of the gas to which people will be exposed. The expert in charge of modeling is facing a major difficulty: few (or no) information. Therefore, for a given situation, the generation of different effect distances is possible.

A sensitivity analysis was carried out in order to determine the most influential parameters on the estimation of safety distances. The goal is to identify the parameters for which it is necessary to pay a very detailed attention.

The first step of the study was to define the system to be analyzed. The second step consisted in working out a complete model of evaluation of safety distances in emergency situation. This was done by combining an existing dispersion model (SLAB) with a specifically developed application for the calculation of input parameters. The input data are operational data which can be collected from the accident site and the output data are safety distances. The third step consisted in selecting two test cases representative of an accident situation involving hazardous chemicals (leak on a wagon of ammonia and a wagon of propane). After that, it was characterizing the range of possible values of the whole input parameters. A fourth step consisted in applying two methods of sensitivity analysis: a screening method (MORRIS's method) and a local sensitivity analysis. Finally, the application of these methods, on the same case study, made it possible to highlight the points of convergence of the methods and their advantages. Finally, the parameters for which it is useless / useful to initiate considerable efforts to recover a reliable value were highlighted.

1. INTRODUCTION

Every day, accidents or pre-accidents involving hazardous materials or chemical processes are managed by Emergency Services. These accidents can cause air pollution. For each phase of an emergency situation (threat, accident, post-accident), in order to bring the best adapted operational answer, it is necessary to determine with accuracy the concentrations of gas to which people will be exposed.

The expert in charge of modeling is facing a major difficulty: few (or no) information to characterize the situation. Therefore, for a given situation, information transmitted (or parameters taken by default in order to complete missing information) may differ dramatically. The result is the generation for a same situation of different effect distances.

An analysis of sensitivity was carried out in order to determine the most influential parameters on the estimation of safety distances. The goal is to identify the parameters for which it is necessary to pay a very detailed attention, either in obtaining a value, or in the choice of a default value, or in its treatment.

The first step of the study was to define the system to be analyzed.

The second step consisted in working out a complete model of evaluation of safety distances in emergency situation. This was done by combining an existing dispersion model (SLAB) with a specifically developed application for the calculation of the input parameters of the dispersion model. The second objective of this model was also to automate calculations for the sensitivity analysis described in the present paper. The input data of the model are operational data which can be collected from the accident site and the output data are safety distances corresponding to effect thresholds. Keeping in mind that this model must be used in emergency situations, three principles were adapted: minimize the number of input data, select methods and models having fast computing times but describing as accurately as possible each physical phenomenon.

The third step consisted in selecting test cases representative of an accident situation involving hazardous chemicals. Two accident scenarios were studied: leak on a wagon of ammonia (toxic liquefied gas) and leak on a wagon of propane (flammable liquefied gas). After that, it was possible to characterize the range of possible or probable values of the whole input parameters needed to make calculations.

A fourth step consisted in applying to this system two methods of sensitivity analysis: a screening method (MORRIS's method) and a local sensitivity analysis.

2. BACKGROUND

2.1 *Methods of sensitivity analysis*

There are mainly three types of methods for sensitivity analysis:

- Screening methods: qualitative methods that reduce the number of input parameters of a model by identifying the most influential parameters on the output [1] [2] [3] [4]. They are used when the number of input parameters is significant in order to reduce the computation time.
- Local sensitivity analysis: quantitative methods based on the calculation of a sensitivity index representative of the model output variations due to a small change of one input parameter [5]. These methods are simple and fast, but appear insufficient to characterize the sensitivity of complex models. Indeed, local sensitivity analysis does not take into account interactions between parameters [6].
- Global sensitivity analysis [7] [8]: quantitative methods for determining the variables that contribute most to the variability of the model response. Unlike local sensitivity analysis, these methods can take into account the density of probability of each input variable and they treat the variation of all parameters simultaneously.

2.2 MORRIS's method

The MORRIS's method [9] [10], better known as the elementary effects method, is the best known screening method. It gives an idea of how the model is answering to potential changes of input parameters. This method allows a rapid identification of influential parameters among a large number of input variables. The influence of each factor input is studied by an approach OAT (One at A Time), that is to say only one factor varies while the others remain fixed. MORRIS's method is useful for identifying potentially influential inputs by dividing them into three groups:

- negligible effects (1)
- linear effects (2)
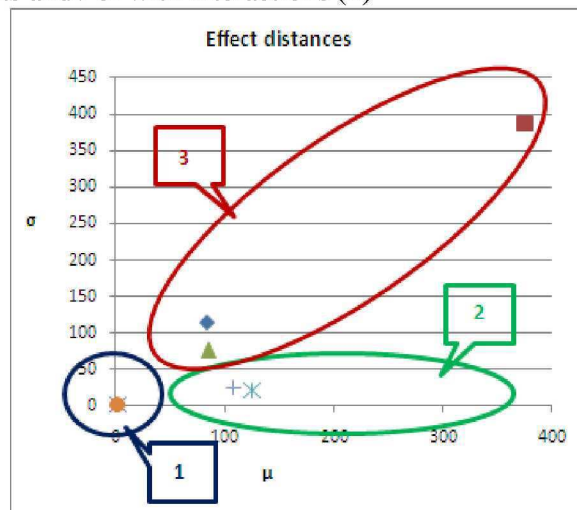- nonlinear effects and / or with interactions (3)

Figure 1 : Example of graph (σ, μ)

To determine these three groups, two sensitivity parameters are provided for each factor input: μ and σ where μ represents the influence of an input factor on the outcome of the model and σ the nonlinear effects and/or the interactions between factors.

$$\mu_i = \frac{1}{r} \sum_{j=1}^{r} d_i\left(X^{(j)}\right) \quad [Eq. 1]$$

$$\sigma_i = \sqrt{\frac{1}{r-1} \sum_{j=1}^{r} (d_i(X^{(j)}) - \mu_i)^2}$$

$$d_i(X) = \frac{Y(X_1, \dots, X_{i-1}, X_i, X_{i+1}, \dots, X_k) - Y(X)}{\Delta}$$

$d_i(X)$ representing the elementary effect of each factor input.

Practically speaking: μ is in fact the mean value of d_i and σ is its standard deviation.

Let k be the number of factors, each varying within *[0 ; 1]*, and p the number of divisions of equal values of the interval *[0, 1/(p-1),...., 1-1/(p-1), 1]*. For each factor, we select r values, generally between 4 and 10, which give r original points. The work of Franco et al [11] showed that with *r = 4* a good ranking of input parameters according to their influence on the final outcome is reached. On the graph below, it can be observed that the relative hierarchy of variables based on the value of μ remains unchanged for a value of r between 4 and 8.
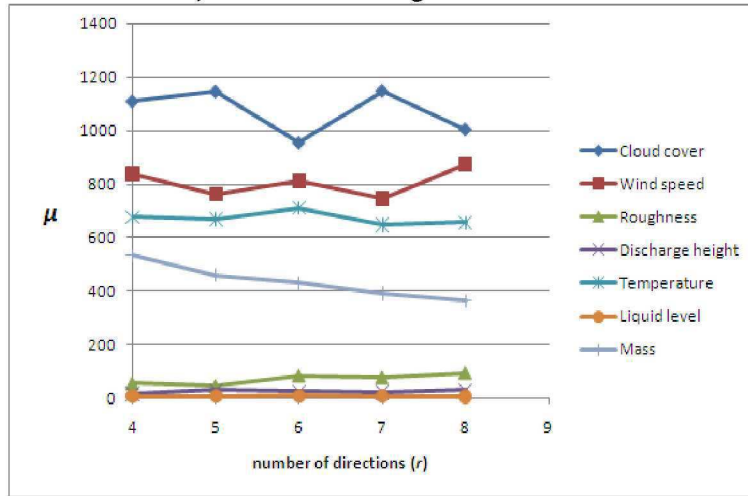

Figure 2 : Evolution of the average influence of variables based

on the number of trajectory (r)

Then, from each of these points, we construct a trajectory by varying the parameters one by one from Δ where *Δ = p / [2 (p-1)]* to ensure an equal probability of sampling in the input space. Each trajectory consists in *(k +1)* points, a factor ranging from Δ at each stage while all others remain fixed. This brings the number of simulations with *n = r (k +1)*.

2.1 Local sensitivity analysis
The local analysis methods are based on the calculation of a sensitivity index showing the variations of model output due to a slight variation of a parameter input. The advantages and disadvantages of these methods have been presented in the following document [12].

Mathematically, consider a model which is written: *$Y = f(X_1, X_2,..., X_k)$* where Y is the response of the model and X_i $i \in [1,...,k]$ are the input parameters, each varying in a given interval with a nominal value X_{i0}. The sensitivity S_i of the response to a low amplitude variation of the parameters Xi corresponds to the partial derivative $S_i = \partial Y / \partial X_i$. For a

complex model, *f* is a function for which we cannot calculate the partial derivatives. Thus, the criterion of sensitivity S_i can be approximated by the expression : $S_i = \Delta Y / \Delta X_i$, where ΔX_i is the difference between the value of X_i in the interval and its nominal value X_{i0}, and ΔY is the difference between the model response at X_i, $Y = f(..., X_i...)$, and the nominal response at X_{i0}, $Y_0 = f(..., X_{i0},...)$, other input parameters are fixed at their nominal value.

However, in order to be able to rank the input parameters according to the model's sensitivity, it is more appropriate to use a dimensionless formulation of the sensitivity criterion, such as: $S_i = (X_{i0}/Y_0)/(\Delta Y/\Delta X_i)$, which is equivalent to calculating the ratio of the relative variations [13].

3. IMPLEMENTATION OF THE METHOD

3.1 Step 1: define the system to be analyzed
The analyzed system can be defined by the definition of its input and output variables:

- Input data: the input data for the analyzed system are **operational data** retrieved from the accident site.

- Output data: the output of the studied system will not be gas concentrations but **effect distances** corresponding to two different effects (lethal and irreversible).
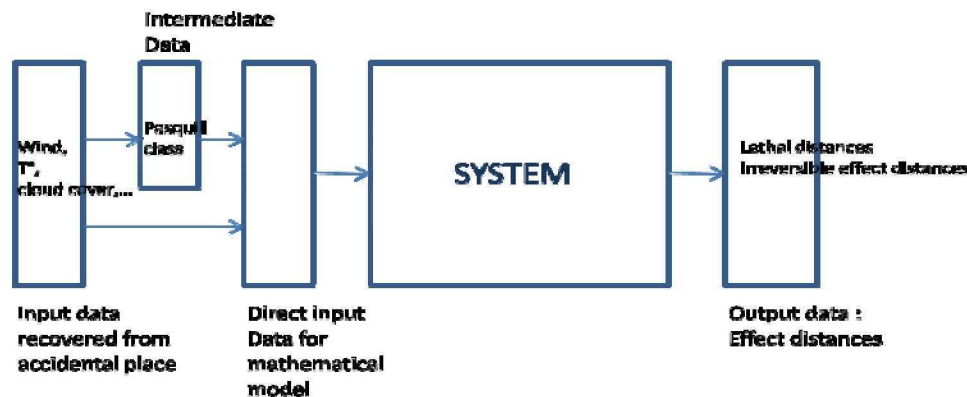

Figure 3 : Characterization of the system to be analyzed

3.2 Step 2: selecting test cases

The principle of sensitivity analysis is to study the model response in a field of input parameters values as large as possible. However, even in this case, it is necessary to fix a number of parameters.

The first one is the chemical. In the case of a leak, two main effects are feared: toxic and explosive effects. It was therefore chosen two fluids: one explosive, the other toxic. This chemical may, under normal conditions, be either liquid or gaseous. In most cases, the mass flow rate generating the cloud is more important in the case of a leak of gas than in a case of liquid layer evaporation. It was therefore decided to study a fluid, which under normal pressure and temperature, is in a gaseous state. Finally, based on the two criteria defined above (type of risk and physical state), the chosen gases must be common enough to be

statistically representative of the toxic and explosive risk. Based on these criteria, it was finally decided to study specifically accidents involving rail transport of **propane** and **ammonia.**

3.3 Step 3.a: working out a complete model of evaluation of safety distances in emergency situation

In order to assess quantitatively the variability of atmospheric dispersion simulations based on input provided by the emergency services, a complete model was built. Keeping in mind that this model should be used in emergency situation, we tried to minimize the number of input data, to select methods and models with time fast calculations. However, selected models will recreate as faithfully as possible the physical phenomena they are supposed to model.

Calculation of input data: mass flow rate

The calculation is done in 3 steps. The first step is to evaluate the mass flow directly out of the release hole (D). The second step is to determine the rate of thermal flash (X). The final step is to determine the rate of spray aerosols $D.(X+K)$.

Evaluation of the initial mass flow rate (D) and thermal flash (X)
There is a low diversity of formulas for evaluating the initial mass flow and initial thermal flash. The initial mass flow rate (D) is evaluated using an evolution of the Bernouilli's formula [14] [15]. The initial thermal flash is determined thanks using a classical isenthalpic expansion formula.

Determination the rate of spray aerosols (K)
It is an uneasily quantifiable parameter. Many empirical methods are offered. These correlations are based on results from observations of experiments with different chemicals and configurations. Each formula should, in theory, be applied only to configurations similar to its development. These formulas are simple to use but very dependent on the rate of thermal flash. Moreover, these methods are mostly independent of the configuration of release (direction, height, pressure). The VTT method [16] was chosen because results from recent and comprehensive testing.

Atmospheric dispersion

The atmospheric dispersion codes can be classified into three categories: Gaussian models, integral models, CFD models. In order to respond quickly with a good scientific level, **integral models** seem currently the most appropriate models according to emergency situation specificities.

SLAB software, available on the website of the U.S. Environmental Protection Agency, meets the requirements of this research work. SLAB is an executable code that reads a text file as input and generates an output text file. This code has no interface which facilitates the automation of calculations.

The SLAB model [17] is an atmospheric dispersion model of integral type, initially based on the concept of air entrainment in a heavy gas cloud and on the effect of subsidence due to its gravity [18]. Coding and computer developments have been made by Ermak and Chan [19]

[17] at the Lawrence Livermore National Laboratory, USA. SLAB can be used for point or surface sources, and for instantaneous or continuous releases. The calculation of the cloud geometrical evolution by SLAB model is shown in figure below. The SLAB model predicts, along the axis of movement, the cloud geometric characteristics (the size of the plan) and concentration fields.
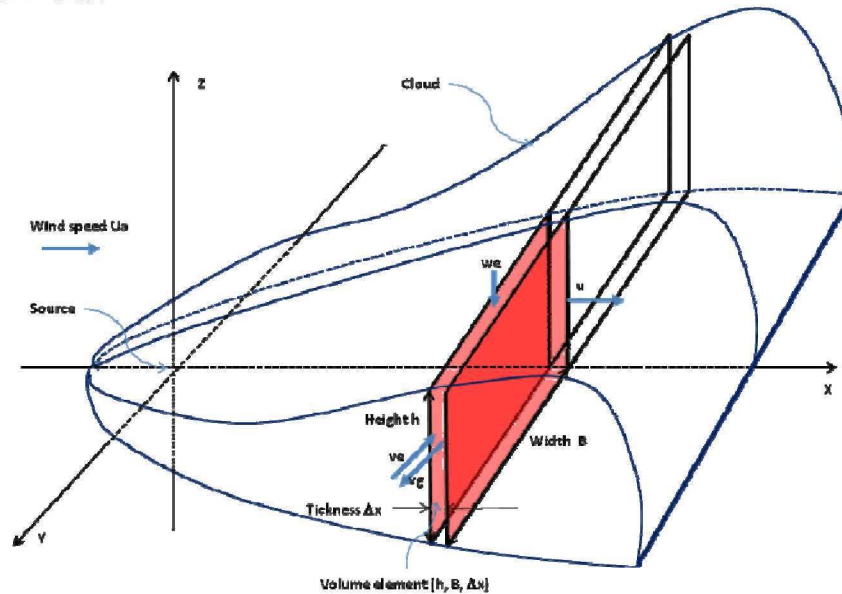

Figure 4 : Calculation of the cloud evolution by the integral method

Calculation of output data: effect distances

The toxic effect distances were obtained by comparison of concentration fields with threshold values for acute toxicity (example: threshold values for acute toxicity or VSTAF in France). The selected effects are irreversible and first lethal effects (LC1%). The overpressure effect distances were obtained by application of the multi-energy method [14].

3.4   Step 3.b: choosing input variables and interval of variation

Based on the constructed model, a minimum list of input data sufficient to describe correctly the situation can be established:

Variable	Unit
Wind speed	m/s
Ambient temperature	K
Stability class	Pasquill
Roughness height	m
Initial mass (or volume) product	kg
Height of product above hole	m
Height of discharge above ground	m
Equivalent radius of hole	m
Product	It is deduced: • The molar mass (and thus gas density) • The density of liquid • The gas and liquid specific heats • The enthalpy of vaporization • The boiling and critical points • The vapor pressure • The ratio of specific heats

Table 1 : List of input variables

In this list, stability class and wind speed are strongly dependent. This dependence is particularly highlighted in the method of estimating the stability class determined by Turner [20]. In order to avoid irrelevant meteorological conditions, we used the method described in the Yellow Book 2nd Edition [21] to determine the sets of meteorological parameters grouped by period of the day and season.

Variable		Interval
Wind speed		[1 m/s ; 9 m/s]
Ambient temperature		Winter : [-5 °C ; 25 °C]
		Summer : [2°C ; 32°C]
		Night : [-5 °C ; 25 °C]
Nebulosity		{0 ; 1 ; 2 ; 3 ; 4 ; 5 ; 6 ; 7 ; 8}
Roughness height		[0,1 m ; 1 m]
Initial mass (or volume) product		[45 m^3 ; 123 m^3]
Height of product above hole		[0 m ; 3 m]
Height of release		[0 m ; 3 m]
Equivalent hole radius		[5 mm ; 80 mm]
Product		
	If flammable : multi-energy index	{3 ; 4 ; 5 ; 6}

Table 2 : Intervals of variation of input variables

3.5   Step 4: coupled sensitivity analysis

It was decided to conduct the sensitivity study using a screening method called MORRIS's method. With a minimum number of experiments, this method allows to assess the sensitivity of each variable on its entire domain.

The results obtained by the MORRIS's method are graphically analyzed. Based on the graphic (μ, σ), it is not trivial to estimate quantitatively the sensitivity of a parameter. That's why the MORRIS's method is coupled with a local sensitivity analysis. This local sensitivity analysis has two objectives: confirm (or invalidate) the sensitivity level of tested parameter, analyze continuity and monotonicity (increasing or decreasing function) of the model response to the input variable tested. The research strategy defined above is illustrated in the following flow chart:
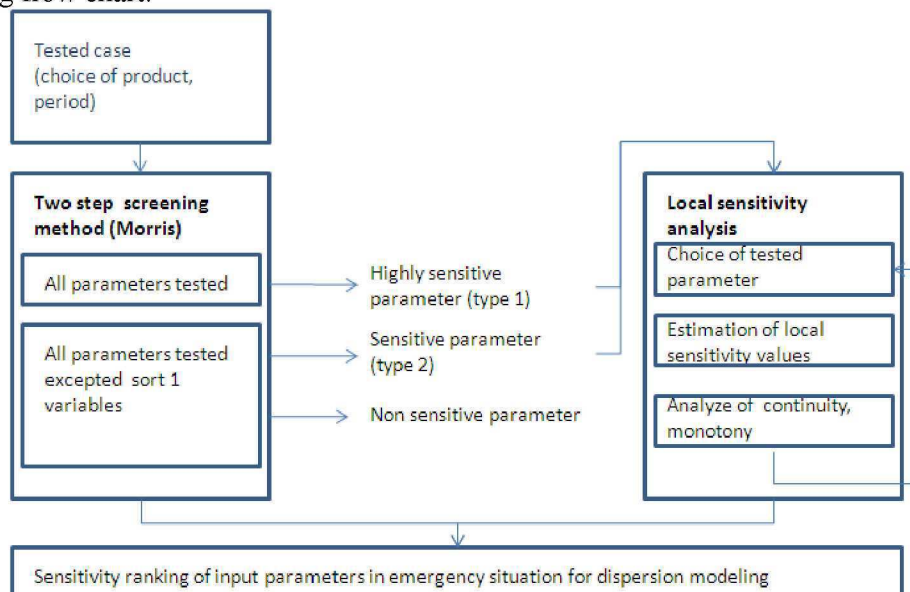
Figure 5 : Flow chart of the sensitivity study

4. RESULTS OF THE SCREENING METHOD

4.1   Screening on all variables

In a first step, a series of tests was conducted using the MORRIS's method with all input variables. A first classification of input parameters according to their influence was established. Globally, it was found that the radius of the hole was the most influential parameter. This first result provides little information as it confirms existing literature [22].
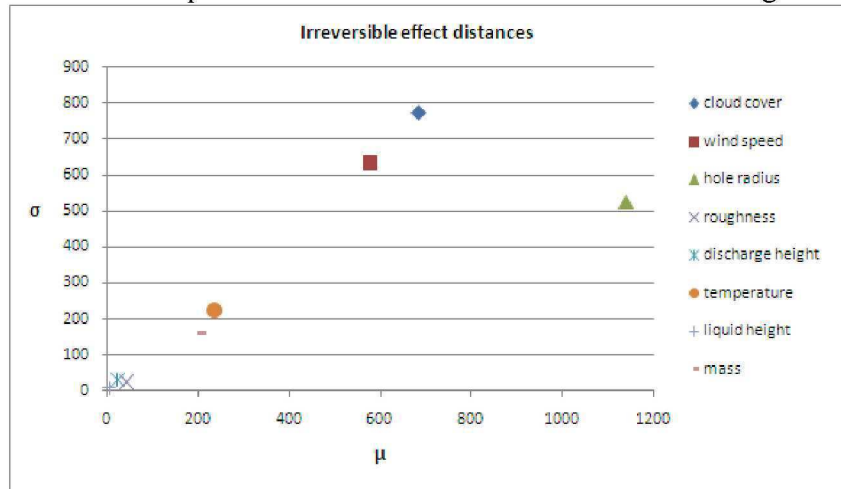
Figure 6 : Graph (σ, µ), ammonia, summer (day), irreversible effects
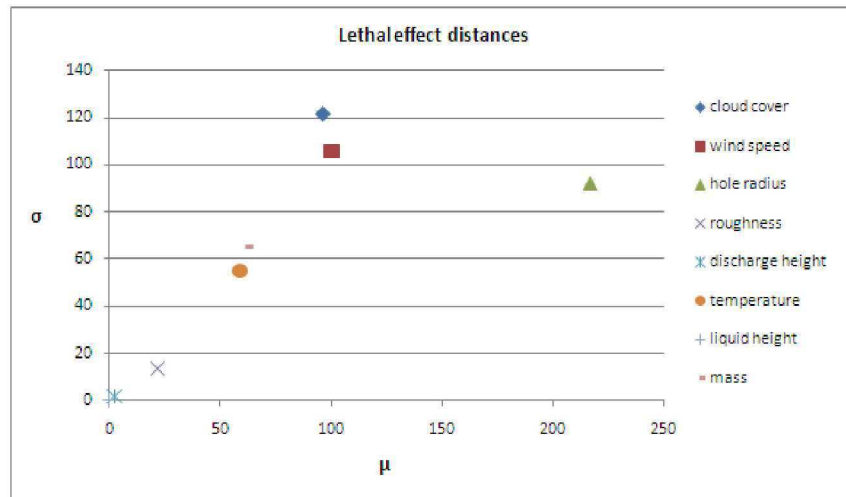
Figure 7 : Graph (σ, µ), ammonia, summer (day), lethal effects

In a second step, the hole radius was excluded from the sensitivity analysis in order to allow the identification of parameters whose influence could be hidden. Two hole radius values were used: the lower bound (representative of a seal leak) and the upper bound (representing a full bore rupture). At each fixed value is corresponding an experimental sub domain. The MORRIS's method is applied to each sub domain.

4.2 Screening with fixed hole radius

4.2.1 Ammonia

A total of six cases have been studied using the MORRIS's method. To each case, the variables listed in table 2 were sampled in their appropriate intervals. These cases are listed below:

Product	Period	Type of Release	Case
Ammonia	Night	Leakage	1
		Rupture	2
	Spring-Summer	Leakage	3
		Rupture	4
	Autumn -Winter	Leakage	5
		Rupture	6

Table 3 : List of sub-cases for ammonia

Examples of graphs (μ, σ) are given below:
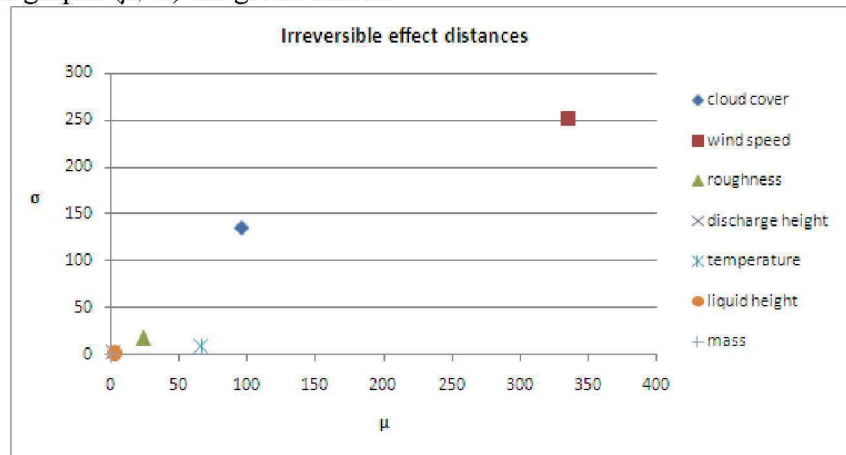
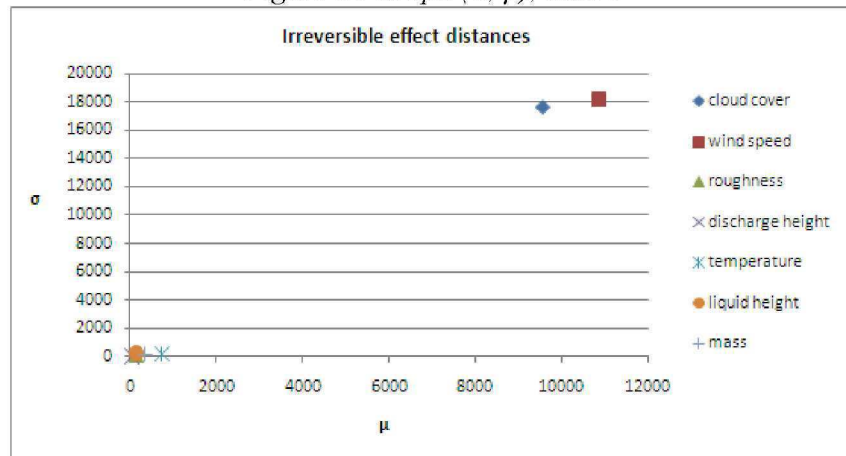*Figure 8 : Graph (σ, μ), case 1*

Figure 9 : Graph (σ, μ), case 2

We calculated μ to classify, for the same case, the parameters into three groups according:

- Green Zone: negligible if $\mu < 1/3 \; \mu_{max}$

- Yellow Zone: not to be overlooked if $1/3 \; \mu_{max} < \mu < 2/3 \; \mu_{max}$

- Red Zone: very influential if $\mu > 2/3 \; \mu_{max}$

The results are shown in the tables below:

NH3 leak	day			night		
	negligible	**not to be overlooked**	**very influential**	**negligible**	**not to be overlooked**	**very influential**
Irrev. Effect Dist.	Mass Release height Liquid height Roughness		Temperature Cloud cover Wind speed	Mass Release height Liquid height Roughness	Temperature Cloud cover	Wind speed
Lethal Effect Dist.	Mass Liquid height Release height	Cloud cover (winter) Wind speed (winter)	Cloud cover (summer) Roughness Temperature Wind speed (summer)	Mass Liquid height Release height	Cloud cover	Temperature Roughness Wind speed

Table 4 : Influence of parameters in case of leakage, NH$_3$

NH3 rupture	day			night		
	negligible	**not to be overlooked**	**very influential**	**negligible**	**not to be overlooked**	**very influential**
Irrev. Effect Dist.	Liquid height Release height Roughness	Temperature (summer) Mass (summer)	Cloud cover Wind speed Temperature (winter) Mass (winter)	Liquid height Temperature Release height	Mass Wind speed	Roughness Cloud cover
Lethal Effect Dist.	Liquid height Release height	Temperature Mass Roughness	Cloud cover Wind speed Temperature	Liquid height Release height Roughness	Mass Temperature Cloud cover	Wind speed

Table 5 : Influence of parameters in case of rupture, NH$_3$

4.2.2   Propane

A total of six cases have been studied using the MORRIS's method. These cases are listed below:

Product	Period	Type of Release	Case
Propane	Night	Leakage	7
		Rupture	8
	Spring-Summer	Leakage	9
		Rupture	10
	Autumn -Winter	Leakage	11
		Rupture	12

Table 6 : List of sub-cases for propane

Examples of graphs (μ, σ) are given below:
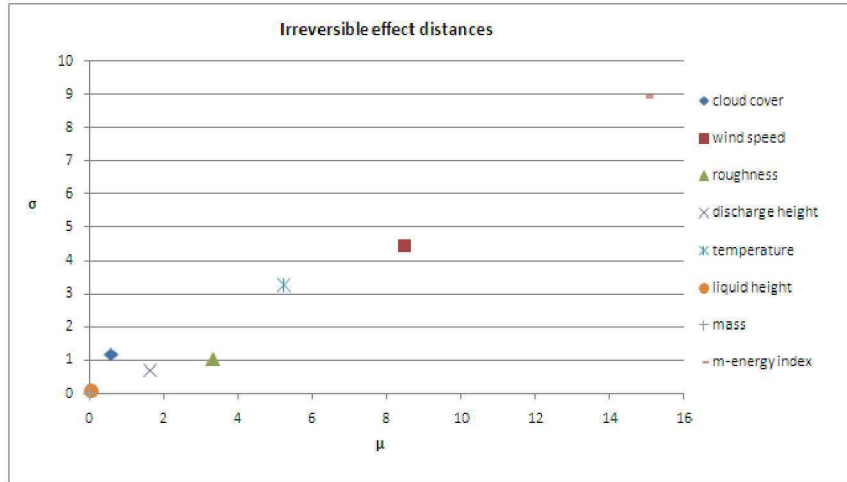
Figure 10 : Graph (σ, μ), case 7
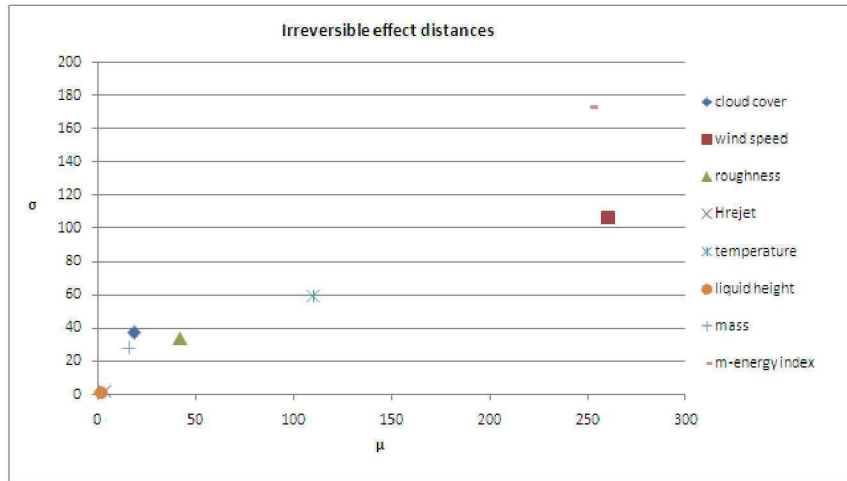
Figure 11 : Graph (σ, μ), case 8

Propane leak	day			night		
	negligible	**not to be overlooked**	**very influential**	**negligible**	**not to be overlooked**	**very influential**
Irrev. Effect Dist. ΔP (50 mbar)	Mass Liquid height Temperature Release height Cloud cover Wind speed Roughness		Multi-energy index	Mass Liquid height Temperature Release height Cloud cover, Roughness	Wind speed	Multi-energy index
Lethal Effect Dist. ΔP (140 mbar)	Mass Liquid height Temperature Release height Cloud cover Wind speed Roughness		Multi-energy index	Mass Liquid height Temperature Release height Cloud cover Wind speed Roughness		Multi-energy index

Table 7 : Influence of parameters in case of leakage, propane

Propane rupture	day			night		
	negligible	not to be overlooked	very influential	negligible	not to be overlooked	very influential
Irrev. Effect Dist. ΔP (50 mbar)	Mass Liquid height Temperature Release height Cloud cover Wind speed Roughness		Multi-energy index	Mass Liquid height Temperature Release height Cloud cover Wind speed Roughness		Multi-energy index
Lethal Effect Dist. ΔP (140 mbar)	Mass Liquid height Temperature Release height Cloud cover Wind speed Roughness		Multi-energy index	Mass Liquid height Temperature Release height Cloud cover Wind speed Roughness		Multi-energy index

Table 8 : Influence of parameters in case of rupture, propane

4.3 Summary of results obtained with the method of screening

The screening method has allowed us to identify unambiguously a certain number of points:

- Height of liquid (above the hole): this parameter, in the case of liquefied gas, has no real importance,
- Discharge height: this parameter, in the case of toxic liquefied gases and within the studied range (0-3 m), has no real influence on the estimate of effect distances. This result is probably due in part to the modeling assumptions. First assumption: in order to take into account the non-prior knowledge of the height of a potential receiver, the concentration of gas at a maximum of 2 m above ground, is evaluated in the axis of the plume. Therefore, within the studied interval of height of release (0 to 3 m), the inhaled concentration is always calculated in the axis of the plume. Second assumption: the empirical formula used for the determination of spray aerosol does not take into the height. In fact, physically, the height of release is influencing this rate. If the release is high, the quantity of liquid on the ground is decreasing (fall time and evaporation time are longer).
- Mass initially contained in the vessel:
  - Flammable gas: the mass contained in the vessel (within the range studied) does not affect the distance effect. The shape of the explosive cloud is stabilizing very quickly (about one minute). Therefore, the duration of leak (and thus the mass of product) has very little influence on the dispersion calculation.
  - Toxic gas: the duration of complete drainage, in case of small leak, is more than an hour (in fact several hours) and, in case of a full bore rupture, is less than one hour (about 15 minutes). The maximal duration of leak is assumed to be equal to one hour (making the assumption that the emergency services can stop the leak in this time interval), the mass contained (within the range studied) is influential in the case of a rupture but not in the case of a leak.
- Meteorological parameters (wind speed, cloud cover, temperature): these variables are always influential. More precisely, the meteorological variables (cloud cover and wind speed in some cases) that enable the estimation of the stability class are more influential than others (temperature and wind speed in other cases).

- Multi-energy index: in the case of a flammable gas, multi-energy index is **THE** most influential parameter.

Other results are equivocal: some parameters, such as roughness height, generate for close configurations very different results. These equivocal results may be due to interactions between parameters.

Beyond these equivocal results, the results, obtained with the MORRIS's method, are analyzed graphically. It is not possible, from the graphics (σ, μ), to estimate quantitatively the sensitivity of a parameter. Therefore, this first analysis is completed for each influential variable with a local sensitivity analysis.

5. RESULTS OF THE LOCAL SENSITIVITY ANALYSIS
5.1 *Construction of experimental design*
Implement local sensitivity analysis requires the information of a vector of input data defining a "optimal" situation. As before, we have considered three distinct periods: summer day, winter day and night.

	Nominal value	Tested values
Nebulosity (-)	3	{1 ; 2 ; 3 ; 4 ; 5 ; 6 ; 7 ; 8}
Wind speed (m/s)	3 m/s	{1 ; 3 ; 4 ; 6 ; 7 ; 9}
Radius (m)	small leak : 0,0025 m rupture : 0,04 m	{0,0025 ; 0,01 ; 0,0175 ; 0,025 ; 0,0325 ; 0,04}
Roughness (m)	0,3 m	{0,10 ; 0,28 ; 0,46 ; 0,64; 0,82 ; 1}
Discharge height (m)	1 m	{0 ; 0,6 ; 1,2 ; 1,8 ; 2,4 ; 3}
Liquid height (m)	0 m	no variation
Temperature (K)	Summer : 290 K Winter : 283 K Night : 283K	Summer: {275 ; 281 ; 287 ; 293 ; 299 ; 305} Winter: {268 ; 274 ; 280 ; 286 ; 292 ; 298} Night: {268 ; 274 ; 280 ; 286 ; 292 ; 298}
Mass (t)	Ammonia : 65 t Propane : 67 t	Ammonia : {55 ; 57 ; 59 ; 61 ; 63 ; 65} Propane : {47 ; 51 ; 55 ; 59 ; 63 ; 67}
Multi-energy index (-)	6 (propane)	{3 ; 4 ; 5 ; 6} (propane)

Table 9 : Table of values used for local analysis

To highlight, for a given variable, the most sensitive areas in its range of values tested, a new sensitivity index S_l is built. The X variables are standardized as follows: $X^* = (X\text{-}X_{min})/(X_{max}\text{-}X_{min})$. For a given parameter, this index is based on the amplitude of the response Y on the entire range tested: $S_l = |(Y(X_{i+1})\text{-}Y(X_i))/(X^*_{i+1}\text{-}X^*_i)).(1/(Y_{max}(X)\text{-} Y_{min}(X)))|$. The interpretation of this parameter is intuitive. Indeed, if we consider an average influence of the tested parameter on its entire range of variation, a part of interval of X with:

- a value of $S_l < 1$ characterizes an area less influential than average,

- a value of $S_l > 1$ characterizes an area more influential than average.

5.2 Ammonia

For each experimental sub-domain, ({ammonia} x {summer (day) ; winter (day) ; night} x {little leak ; rupture}), the evolution of effect distances and local sensitivity indices based on the variation of each input parameter were estimated. Examples of results obtained are given below:
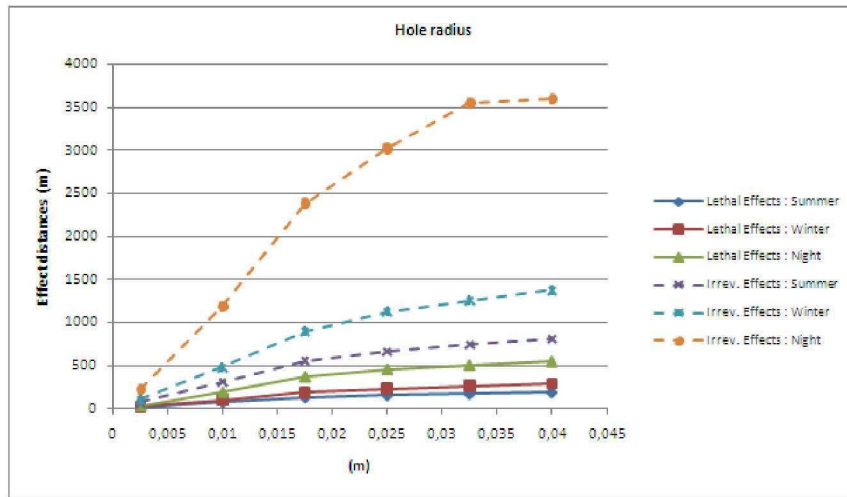

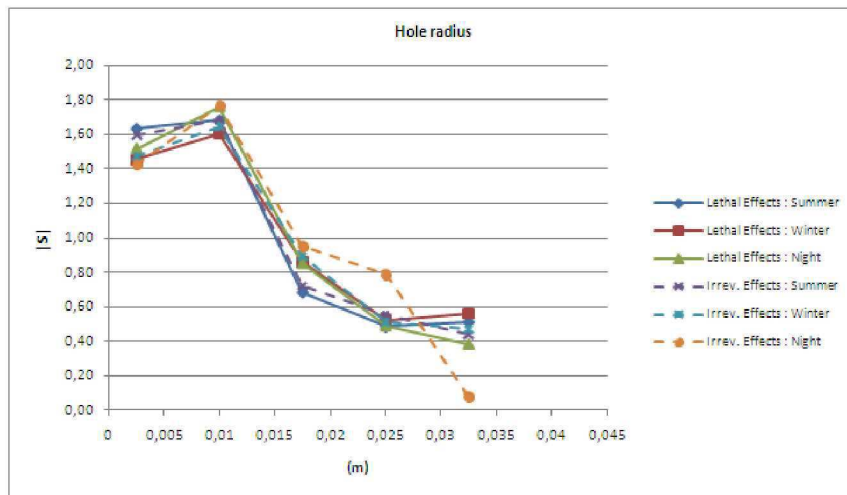*Figure 12 : Ammonia, radius variation, effect distances*

Figure 13 : Ammonia, radius variation, sensitivity index

According to figures 12 and 13, it appears that hole size has a monotonically increasing influence on the effect distances. Its influence is decreasing beyond a threshold between 10 and 15 mm. One explanation is possible: for a given initial mass, if the radius is increasing, the release rate is increasing but the duration of discharge is decreasing. The dose calculation is incurring a double contradictory influence.
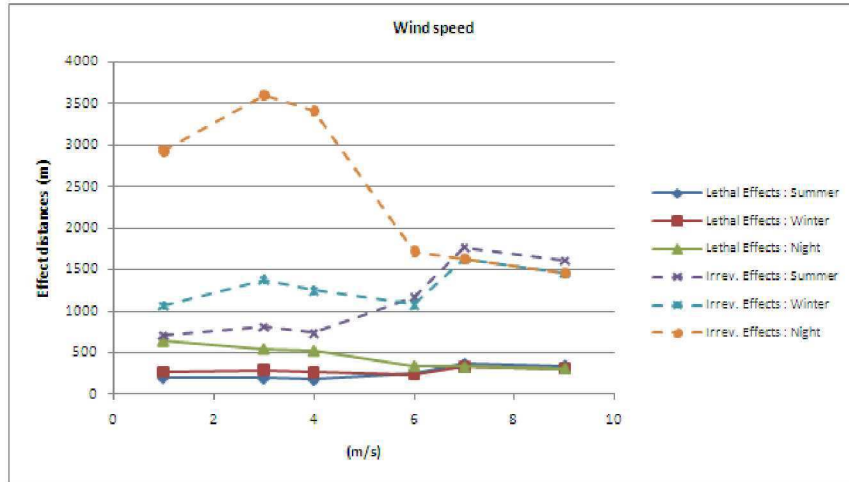
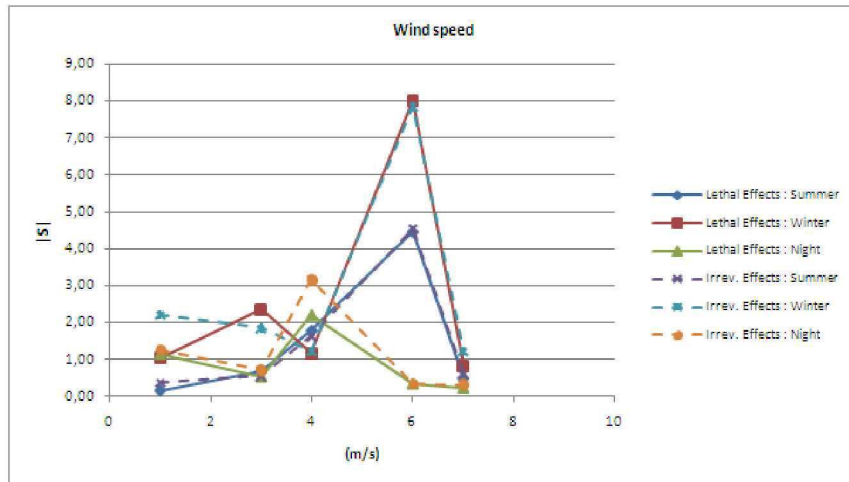*Figure 14 : Rupture, ammonia, wind speed variation, effect distances*

Figure 15 : Rupture, ammonia, wind speed variation, sensitivity index

According to figures 14 and 15, it appears that wind speed has globally an increasing influence during the day (increasing stability) and a decreasing influence during the night (decreasing stability and increasing cloud dilution). Specifically, during the day, it appears that an increase of wind speed generates two conflicting effects: increasing the stability, which leads to increased effect distances, and increasing the dilution, which leads to decreased effect distances. For wind speeds above 6 m/s, the stability classes remaining constant (D for day and night), the influence of wind is negligible.

5.3   Propane
The same work was done for propane. It will be presented in detail in a future paper. Among the main results, we can mention the predominant effect of the choice of the multi-energy index.

5.4   Summary of results obtained with local sensitivity analysis
Local sensitivity analysis has enabled to:
- Characterize, for a given variable, how the distance is influenced by this variable:
  - monotonic / non-monotonic function (example : roughness for ammonia),
  - continuous / non-continuous function (example: cloud cover),

o constant influence (example: temperature) / non-constant (example: multi-energy index).
- Evaluate, in an easily understandable way, the magnitude of possible changes in results due to variation of one input parameter (example: lethal effect distances with multi-energy index of 6 / lethal effect distances with multi-energy index of 3 = +∞).
- Confirm the existence of variables with a complex influence on the final result (example: roughness height). There are probably interactions between this variable and other input variables or with the concentration value associated with the desired effect.

6. DISCUSSION AND CONCLUSION

The two cases studied were an accident on wagon carrying ammonia or propane (**toxic liquefied gas / flammable liquefied gas**).

The sensitivity analysis has allowed the detection of certain types of influence on the final result:
- **Never influential variables:**
  o <u>Liquid height</u>: Logical result because the flow in the case of LPG, mainly depends on internal pressure and not on hydrostatic pressure.
  o <u>Release height (above 1 m)</u>: Logical result according to the chosen computational hypothesis. Between 0 and 1 m, the sensitivity is increased probably due to an interaction of release height with the roughness height.
- **Always very influential variables:**
  o <u>Wind speed</u> and <u>cloud cover</u>. These two parameters are always very influential. Indeed, the wind speed is an important factor in the mechanism of atmospheric dispersion. But it is also involved in determining the atmospheric stability class in combination with the cloud cover.
  o <u>Multi-energy index</u> for flammable gas.
- **Always influential variables**: <u>Temperature</u>. Temperature is always influential and has an increasing influence on effect distances. The most likely explanation is that in case of a liquefied gas, for a same hole (shape, size and location) the mass flow is mainly depending on the internal pressure. In the case of transportation of LGP, this internal pressure can be assimilated to the saturated vapor pressure which is very sensitive (globally increasing exponentially) to the fluid temperature (equal to ambient temperature in our case).
- **Influential but not decisive variables:** <u>Total initial mass in the vessel</u>. For a flammable gas, the total mass of fluid in the vessel has no influence (within the range studied). This is due to the fact that the shape of gas cloud is reaching very fast its steady state. For toxic gas, if the maximal duration of leak is assumed to be equal to one hour (to take into account the response time of emergency services), the mass contained (within the range studied) is influential in the case of a full bore rupture but not in the case of a leak.
- **No monotonic influence variables:** <u>Roughness</u>. It was not possible to highlight a simple behavior of the model in function of the roughness value (which however has not a negligible influence).

The sensitivity analysis has another interest: it allows the detection of implicit assumptions used by the software (example: rain-out independent of the height of release). For a model of

the same family, we can assume that the classification of the input variables according to their influence would be identical to that presented in this article.

This work is allowing the development of a first operational classification of input variables:
- **Variables with little or no influence** for which it is possible to set a fixed value by default (example: height of liquid above the hole).
- **Influential variables** for which :
  o A precise value can be obtained easily (example: wind speed, temperature).
  o The recovery of value can (or must) be improved (example: cloud cover).
  o A deterministic approach may not be satisfactory. These are the variables for which the recovery of a reliable value is very difficult (example: size of gap) or with a non monotonic influence (example: roughness). For these variables, a possible solution might be to use intervals of expected values and simulate a suitable set of cases. A final step would be to provide to the crisis manager an operational result on the basis of all modeling performed.

Finally, future developments can be proposed like, for example, an extension of the experimental field for the local sensitivity analysis. Some areas of variations could be reviewed (example: minimum temperature closer to the boiling temperature of the product).

7. REFERENCES

[1] Bettonvil, B. & Kleijnen, J. P. Searching for important factors in simulation models with many factors: Sequential bifurcation European Journal of Operational Research, 1997, 96, 180-194

[2] Campolongo, F. & Braddock, R. The use of graph theory in the sensitivity analysis of the model output: a second order screening method Reliability Engineering & System Safety, 1999, 64, 1-12

[3] Deana, A. M. & Lewis, S. M. Comparison of group screening strategies for factorial experiments Computational Statistics & Data Analysis, 2002, 39, 287 – 297

[4] Morris, M. D. Input screening: Finding the important model inputs on a budget Reliability Engineering & System Safety, 2006, 91, 1252-1256

[5] Turányi, T. & Rabitz, H. Local Methods, in : Sensitivity Analysis John Wiley & Sons Publication, 2004

[6] Saltelli, A. & Annoni, P. How to avoid a perfunctory sensitivity analysis Environmental Modelling & Software, 2010, 25, 1508 - 1517

[7] Saltelli, A.; Chan, K. & Scott, E. Sensitivity Analysis Wiley, 2000

[8] Jacques, J. Contributions à l'analyse de sensibilité et à l'analyse discriminante généralisée Université Joseph Fourier - Grenoble 1, 2005

[9] Morris, M. D. Factorial Sampling Plans for Preliminary Computational Experiments Technometrics,, 1991, 33, 161-174

[10] Campolongo, F.; Cariboni, J. & Saltelli, A. An effective screening design for sensitivity analysis of large models Environmental Modelling & Software, 2007, 22, 1509 - 1518

[11] Francos, A.; Elorza, F. J.; Bouraoui, F.; Bidoglio, G. & Galbiati, L. Sensitivity analysis of distributed environmental simulation models: understanding the model behaviour in hydrological studies at the catchment scale Reliability Engineering & System Safety, 2003, 79, 205 - 218

[12] Frey, H. C. & Patil, R. S. Identifcation and review of sensitivity analysis methods Risk Analysis, North Carolina State University, 2002, 553-578

[13] Chokmani, K.; Viau, A. A. & Bourgeois, G. Analyse de l'incertitude de quatre modèles de phytoprotection relative à l'erreur des mesures des variables agrométéorologiques d'entrée Agronomie, 2001, 21, 147-167

[14] RIVM Yellow book - Methods for the calculation of physicals effects - CPR 14E TNO, 2005

[15] UIC Emission à la brèche d'une capacité débit en phase gazeuse débit en phase liquide formation et vaporisation des flaques UIC, 1987

[16] Lautkaski, R. Experimental correlations for the estimation of the rainout of flashing liquid releases—Revisited Journal of Loss Prevention in the Process Industries, 2008, 21, 506 - 511

[17] Ermak, D. User's Manual for SLAB: An atmospheric dispersion model for denser-than-air releases Lawrence Livermore National Laboratory, 1990

[18] Zeman, O. The dynamics and modeling of heavier-than-air, cold gas releases Atmospheric Environment (1967), 1982, 16, 741 - 751

[19] Ermak, D.; Rodean, H.; Lange, R. & Chan, S. A survey of denser-than-air atmospheric dispersion models Lawrence Livermore National Laboratory, 1988

[20] Turner, D. B. Workbook of Atmospheric Dispersion Estimates EPA Office Air Prog. Rep, 1970, AP-26

[21] RIVM Yellow book - Methods for the calculation of physicals effects - CPR 14E TNO, 1992

[22] Pandya, N. Analyse de sensibilité paramétrique d'un outil de modélisation des conséquences de scénarios d'accidents. Application à la dispersion atmosphérique de rejets avec le logiciel Phast. Institut National Polytechnique de Toulouse, 2009