Sensitivity Analysis in presence of model uncertainty and correlated inputs

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Abstract

The first motivation of this work is to take into account model uncertainty in sensitivity analysis. We present with some examples, a methodology to treat uncertainty due to a mutation of the studied model. Development of this methodology has highlighted an important problem, frequently encountered in sensitivity analysis: how to interpret sensitivity indices when random inputs are non-independent? This paper suggests a strategy for the problem of sensitivity analysis of models with non-independent random inputs. We propose a new application of the multidimensional generalization of classical sensitivity indices, resulting from group sensitivities (sensitivity of the output of the model to a group of inputs), and describe an estimation method based on Monte-Carlo simulations. Practical and theoretical applications illustrate the interest of this method.

Key words: Global sensitivity analysis, model uncertainty, model mutation, correlated inputs, multidimensional sensitivity indices.

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1 Introduction

In many fields like structural reliability, behavior of thermohydraulic systems, or nuclear safety, mathematical models are used for simulation, when experiments are too expensive or even impracticable, and for prediction. In this context, sensitivity analysis (SA) tries to answer the following question: how does the output depend on its uncertain inputs? Application for SA are model calibration or model validation, and decision making process, where it is generally very useful to know which variables mostly contribute to output variability. We distinguish two classes in sensitivity analysis: local SA and global SA. Local SA studies how little variations of inputs around a given value change the value of the output. Global SA takes into account all the variation range of the inputs, and tries to apportion the output uncertainty to the uncertainty in the input factors. We review quickly in Section 2 a class of global sensitivity analysis methods based on decomposing the variance output.

The purpose of our works is to take into account a type of model uncertainty in sensitivity analysis, which is often encountered in practice: consider that a model, on which sensitivity analysis has been made is subsequently modified. In this case, is it possible to obtain information about sensitivity analysis of the transformed model, without doing a new complete sensitivity analysis, but by using instead results obtained from the original model? In the Section 3, we present some useful strategies to answer this question. For some possible mutations, sensitivity indices of the transformed model can be formally related to those of original model. We also present in Section 4, a new application of group sensitivities (sensitivity of the output of the model to a group of inputs), for models with non independent input factors.

2 Variance based sensitivity measures

Among global sensitivity analysis techniques, variance based methods are the most often used. The main idea of these methods is to express sensitivity through variance, and to evaluate how the variance of such an input or group of inputs contributes into variance of the output.

Consider the following model:

$$\begin{aligned} f : \mathbb{R}^p &\rightarrow \mathbb{R} \\ \mathbf{X} &\mapsto Y = f(\mathbf{X}), \end{aligned} \tag{1}$$

where Y is the output, $\mathbf{X} = (X_1, \ldots, X_p)$ are p independent inputs, and f is the model function, which can be analytically not known.

An indicator of the importance of an input X_i could be based on what would the variance of Y be if we fix X_i to its true value x_i^*: $V(Y|X_i = x_i^*)$. This quantity is the conditional variance of Y given $X_i = x_i^*$. But in most cases, the true value x_i^* of X_i is not known. To solve this problem, the average of this conditional variance under all possible values for x_i^*, noted $E[V(Y|X_i = x_i^*)]$, is studied. Using the following property:

$$V(Y) = V(E[Y|X_i = x_i^*]) + E[V(Y|X_i = x_i^*)],$$

$V(E[Y|X_i = x_i^*])$ is used like an indicator of the importance of X_i on the variance of Y, or of the sensitivity of Y to X_i. This quantity, named *variance of the conditional expectation* and generally noted $V(E[Y|X_i])$, has an important property: the greater the importance of X_i, the greater is $V(E[Y|X_i])$. Finally, to have a normalized indicator between 0 and 1, the used sensitivity index is defined by:

$$\frac{V(E[Y|X_i])}{V(Y)}. \tag{2}$$

This indicator is named *first order sensitivity index* by Sobol [1], *correlation ratio* by McKay [2], or *importance measure* by Ishigami and Homma [3]. It measures the main effect of X_i on the output Y.

Sobol [1] has introduced this index in decomposing the model function f into summands of increasing dimensionality:

$$f(x_1, \ldots, x_p) = f_0 + \sum_{i=1}^{p} f_i(x_i) + \sum_{1 \leq i < j \leq p} f_{ij}(x_i, x_j) + \ldots + f_{1 \ldots p}(x_1, \ldots, x_p), \tag{3}$$

where functions of the decomposition have two important properties: their integrals over any of its own variables are zero, and they are mutually orthogonal.

Thus, this decomposition leads to the following decomposition of the variance of Y:

$$V(Y) = \sum_{i=1}^{p} V_i + \sum_{1 \leq i < j \leq p} V_{ij} + \ldots + V_{1\ldots p}, \tag{4}$$

where:

$$\begin{aligned}
V_i &= V(E[Y|X_i]) \\
V_{ij} &= V(E[Y|X_i, X_j] - E[Y|X_i] - E[Y|X_j]) \\
V_{ijk} &= V(E[Y|X_i, X_j, X_k] - E[Y|X_i, X_j] - E[Y|X_i, X_k] - E[Y|X_j, X_k] \\
&\quad + E[Y|X_i] + E[Y|X_j] + E[Y|X_k]),
\end{aligned}$$

and so on.

As all inputs are assumed to be independent, we have:

$$\begin{aligned}
V_i &= V(E[Y|X_i]) \\
V_{ij} &= V(E[Y|X_i, X_j]) - V_i - V_j \\
V_{ijk} &= V(E[Y|X_i, X_j, X_k]) - V_{ij} - V_{ik} - V_{jk} - V_i - V_j - V_k.
\end{aligned}$$

From this decomposition, first order sensitivity indices are defined by $S_i = \frac{V_i}{V(Y)}$ like in (2), second order sensitivity indices by $S_{ij} = \frac{V_{ij}}{V(Y)}$, and so on. The second order index S_{ij} expresses sensitivity of the model to the interaction between X_i and X_j: the part of the variance of Y due to X_i and X_j which is not included in the individual effects of X_i and X_j. It is also possible to define higher order indices.

The sum of all order indices is equal to 1, if all input variables are independent.

So, in this case, index values are easy to interpret: the greater an index value, the greater is the importance of the variable or of the group of variables, that is linked to this index.

For a model with p inputs, the number of all order indices is $2^p - 1$. As this number can be very important when p increases, total sensitivity indices have been introduced by Homma and Saltelli in [4]. For an input X_i, the total sensitivity index S_{T_i} is defined as the sum of all indices relating to X_i (first and higher order). For example, for a model with $p = 3$ inputs, $S_{T_1} = S_1 + S_{12} + S_{13} + S_{123}$.

One method of estimation of these indices is introduced by Sobol [1], using Monte-Carlo simulations. Saltelli extends this method for a best use of model evaluations, and also for lower cost [5]. Another method, named FAST (*Fourier Amplitude Sensitivity Test*) is also defined by Cukier et al.[6] and Schaibly and Shuler [7], and extended for total indices by Saltelli et al. [8].

For more information on variance based sensitivity measures, refer to [9].

3 Impact of model uncertainty on sensitivity analysis

Assume that a sensitivity analysis have been made on a model $M : Y = f(X_1, ..., X_p)$, where the p input variables X_i are independent. Let us suppose that new informations about the model, new measurements, or even changes in the modelized process, oblige us to consider a new model M_{mut}, that is also a mutation of the original model M. Let us present some mutations, for which interesting results have been obtained. In the first one, a random variable is fixed to a given value. In the second one, we consider that we have made two sensitivity analyses on two models, and that we decide to study the sum of this two models.

A random input becomes deterministic. Suppose that a variable X_i from a given model $Y = f(X_1, ..., X_i, ..., X_p)$ is fixed to α (in practice we have most of the time $\alpha = E[X_i]$, but not necessarily). Is it possible to compute the new sensitivity indices of the mutated model $Y' = f(X_1, ..., \alpha, ..., X_p)$ from the sensitivity indices of $Y = f(X_1, ..., X_i, ..., X_p)$? To answer this question, assumptions on the shape of the function f are needed.

(i) Assume that $Y = \sum_{k=1}^{n} f_k^1(X_i) f_k^2(\vec{X}_{\sim i})$, where $\vec{X}_{\sim i} = (X_1, ..., X_{i-1}, X_{i+1}, ..., X_p)$ is the input vector without the variable X_i. The conditional expectation of Y given a variable X_j $(j \neq i)$ can be linked to the conditional expectation of Y' given X_j by: $E[Y'|X_j] = E[Y|X_j] + \sum_{k=1}^{n}(E[f_k^1(\alpha)] - E[f_k^1(X_i)])E[f_k^2(\vec{X}_{\sim i})|X_j]$. If we make further the hypothesis that the functions f_k^1, for $1 \leq k \leq n$, are linear, *i.e.* $f_k^1(t) = at+b$, and if $\alpha = E[X_i]$, then first and higher order sensitivity indices S' of Y' can be obtain from sensitivity indices S of Y by:

$$S' = S \times \frac{V(Y)}{V(Y')}. \tag{5}$$

Proof. We have

$$\begin{aligned} E[Y^{'}|X_j] &= E[Y|X_j] + \sum_{k=1}^{n} (\underbrace{E[a\alpha+b]-E[aX_i+b]}_{a\alpha+b-(aE[X_i]+b)}) E[f_k^2(\vec{X}_{\sim i})|X_j] \\ &= E[Y|X_j] \quad \text{because } E[X_i]=\alpha, \end{aligned}$$

and so:

$$\frac{V(E[Y^{'}|X_j])}{V(Y')} = \frac{V(E[Y|X_j])}{V(Y)} \times \frac{V(Y)}{V(Y')}.$$

$\square$

Note that all indices relating to the variable X_i disappear. For total indices, if they have been computed by the sum of all order indices, we can also obtain them by (5). Effectively, all order indices of the transformed model $Y^{'}$ can be obtained by (5), and so we just have to compute their sum to obtain total indices of $Y^{'}$. If not, they must be estimated by a new analysis.

(ii) Assume now that $Y = f_1(X_i) + f_2(\vec{X}_{\sim i})$. In this case we can omit the assumption of linearity of f_1. Then, as $E[Y|X_j] = E[f_1(X_i)] + E[f_2(\vec{X}_{\sim i})|X_j]$ and $E[Y^{'}|X_j] = f_1(\alpha) + E[f_2(\vec{X}_{\sim i})|X_j]$, we have $V(E[Y^{'}|X_j]) = V(E[Y|X_j])$, and we can thus obtain sensitivity indices $S^{'}$ of $Y^{'}$ from sensitivity indices S of Y by (5). This formula is right for all order and total order indices too, because, in the model Y, all sensitivity indices $S_{i,j}$ are equal to 0 (for all $j \neq i$). This is due to the fact that X_i is not in interaction with other variables. Like in first case, all indices relating to the variable X_i disappear.

(iii) Assume finally that $Y = f_1(X_i)f_2(\vec{X}_{\sim i})$. Like conditional expectation of Y and $Y^{'}$ given X_j are $E[Y|X_j] = E[f_1(X_i)]E[f_2(\vec{X}_{\sim i})|X_j]$ and $E[Y^{'}|X_j] = f_1(\alpha)E[f_2(\vec{X}_{\sim i})|X_j]$, we have $V(E[Y^{'}|X_j]) = \frac{f_1(\alpha)^2}{E[f_1(X_i)]^2}V(E[Y|X_j])$. First and higher order sensitivity indices $S^{'}$ of $Y^{'}$ can also be obtained from sensitivity indices S of Y by:

$$S^{'} = S \times \frac{V(Y)}{V(Y')} \times \frac{f_1(\alpha)^2}{E[f_1(X_i)]^2}, \tag{6}$$

and all indices relating to the variable X_i disappear. For total indices, like in the case (i), if they have been estimated for Y like the sum of all order indices, we can obtain those of $Y^{'}$ by (6), else, a new analysis is needed.

Sum of two models. Consider two models Y_1 and Y_2, and assume that sensitivity analysis have been made on each model, and so that sensitivity indices S^1 for Y_1 and S^2 for Y_2 have been computed. How can sensitivity indices S^Y of $Y = Y_1 + Y_2$ be obtained?

(i) Assume first that all input variables are different for Y_1 and Y_2, i.e. $Y_1 = f_1(X_1, ..., X_p)$ and $Y_2 = f_2(X_{p+1}, ..., X_{p+q})$. We suppose that these inputs are independent. The conditional expectation of Y given X_j, is equal to $E[Y_1|X_j] + E[Y_2]$ if $1 \leq j \leq p$ or to $E[Y_2|X_j] + E[Y_1]$ if $p+1 \leq j \leq p+q$. The terms $E[Y_2]$ and $E[Y_1]$ are constant, and so $V(E[Y_1|X_j]+E[Y_2]) = V(E[Y_1|X_j])$ and $V(E[Y_2|X_j] + E[Y_1]) = V(E[Y_2|X_j])$. Thus, sensitivity indices of Y can be obtained by multiplying those of Y_1 by $\frac{V(Y_1)}{V(Y_1)+V(Y_2)}$ and those of Y_2 by $\frac{V(Y_2)}{V(Y_1)+V(Y_2)}$. It is easy to verify that all sensitivity indices, relative to interaction between variables of Y_1 and Y_2 are equal to zero.

(ii) Assume now that the two models have the same input variables, the conditional expectation of Y given a variable X_j is equal to the sum of the conditional expectation of Y_1 given X_j and the conditional expectation of Y_2 given X_j. Thus, the first order sensitivity indices of Y are linked to those of Y_1 and Y_2 by:

$$S_j^Y = S_j^1 \times \frac{V(Y_1)}{V(Y)} + S_j^2 \times \frac{V(Y_2)}{V(Y)} + \frac{2\mathrm{Cov}(E[Y_1|X_j], E[Y_2|X_j])}{V(Y)}.$$

But the estimation of the covariance is in practice as expensive as direct estimation of sensitivity indices of Y.

(iii) Assume finally, that the two models have common and different variables. We can also obtain from analysis of Y_1 and Y_2, only sensitivity indices relating to variables which belong to only one of the two models. Effectively, if $Y_1 = f_1(X_1, ..., X_p)$ and $Y_2 = f_2(X_1, ..., X_{p+q})$, same type of calculus allows one to obtain sensitivity indices relating to variables $(X_{p+1}, ..., X_{p+q})$, by multiplying sensitivity indices of Y_2 by $\frac{V(Y_2)}{V(Y)}$.

We will see an application of those results, which we will name thereafter *mutation method*, in the Section 5.

4 Multidimensional sensitivity analysis using group sensitivities

In the Section 2 and 3, it has been assumed that input variables were independent. But in practice, this assumption is sometimes difficult to justify.

The problem when inputs are correlated concerns the interpretation of sensitivity indices values. We have seen in Section 2, that, when inputs are independent, the sum of all sensitivity indices is equal to 1. If we don't assume that inputs are independent, functions of Sobol decomposition (3) are not orthogonal, and so a new term appears in the variance decomposition (4). This term implies that the sum of all order sensitivity indices is not equal to 1. Effectively, variabilities of two correlated variables X_i and X_j are linked, and so when we quantify sensitivity to one of this two variables, we also quantify a part of sensitivity due to the other variable. It is always possible to compute $V(E[Y|X_i, X_j])$, but we are no longer capable of decomposing it in first order effect, $V(E[Y|X_i])$ and $V(E[Y|X_j])$, and interaction effect, $V(E[Y|X_i, X_j] - E[Y|X_i] - E[Y|X_j])$. A straightforward solution is to define multidimensional or group sensitivity indices for groups of correlated variables.

This possibility of applying sensitivity analysis to a group internally correlated but not across is already known ([1]), but we have not seen applications in the literature. We propose here an interesting one to the case of models with correlated inputs.

Consider the model $Y = f(\mathbf{X})$, defined in (1), and assume that the covariance matrix of $\mathbf{X}$ is not a diagonal matrix, *i.e.* such variables are correlated with others. Assume that all variables are not correlated, but there are groups of correlated inputs. Variables into a group are dependent, but variables of different groups are independent. We note each group like a multidimensional variable $\vec{X}_i$. The p-dimensional input $\mathbf{X}$ can also be written:

$$\mathbf{X} = (\underbrace{X_1}_{\vec{X}_1}, ..., \underbrace{X_I}_{\vec{X}_I}, \underbrace{X_{I+1}, ..., X_{I+k_1}}_{\vec{X}_{I+1}}, \underbrace{X_{I+k_1+1}, ..., X_{I+k_2}}_{\vec{X}_{I+2}}, ..., \underbrace{X_{I+k_{L-1}+1}, ..., X_p}_{\vec{X}_{I+L}}).$$

One-dimensional non independent variables $(X_1, ..., X_p)$ are written like multidimensional independent variables $(\vec{X}_1, ..., \vec{X}_{I+L})$. We propose to define sensitivity indices, like in classical case of independent inputs. Thus, first order sensitivity indices are defined by:

$$S_j = \frac{V(E[Y|\vec{X}_j])}{V(Y)} \quad \forall j \in [1, I+L].$$

This index measures the impact of the multidimensional variable $\vec{X}_j$ on the output Y. To connect this to one-dimensional variables, if the variable $\vec{X}_j$ is one-dimensional (case where $j \in [1, ..., i]$), we have well defined the same index:

$$S_j = \frac{V(E[Y|\vec{X}_j])}{V(Y)} = \frac{V(E[Y|X_j])}{V(Y)},$$

and if its dimension is larger than 1 (case $j \in [I+1, ..., I+L]$ for example $j = I+2$), the index is defined by the variance of conditional expectation of Y given $\vec{X}_j = (X_{I+k_1+1}, ..., X_{I+k_2})$:

$$S_j = S_{\{I+k_1+1,...,I+k_2\}} = \frac{V(E[Y|X_{I+k_1+1}, ..., X_{I+k_2}])}{V(Y)}.$$

We can also define higher order indices and total sensitivity indices. Second order indices are given by:

$$S_{jk} = \frac{V(E[Y|\vec{X}_j, \vec{X}_k] - E[Y|\vec{X}_j] - E[Y|\vec{X}_k])}{V(Y)}.$$

This index expresses sensitivity of Y to interaction between multidimensional inputs $\vec{X}_j$ and $\vec{X}_k$, and so on for higher order indices. Finally, total order indices can be defined by: $S_{T_j} = \sum_{k\#j} S_k$, where $\#j$ represents all subsets of

$\{1, ..., I+L\}$ which include j.

It is very important to note that if all input variables are independent, all groups contain only one variable, and so those group sensitivity indices are clearly the same than those defined in Section 2 for independent inputs.

4.1 Numerical estimation

We present a simple way of estimation of those multidimensional sensitivity indices, based on the Sobol estimation method, applying Monte-Carlo simulations.

Firstly, we estimate mean of Y by $\hat{f}_0 = \frac{1}{N}\sum_{k=1}^{N} f(\vec{x}_1^k, ..., \vec{x}_{I+L}^k)$ and variance by $\hat{D} = \frac{1}{N}\sum_{k=1}^{N} f^2(\vec{x}_1^k, ..., \vec{x}_{I+L}^k) - \hat{f}_0^{\ 2}$ where $(\vec{x}_1^k, ..., \vec{x}_{I+L}^k)_{k=1,N}$ is a set of N simulations of multidimensional inputs.

First order indices are estimated by $S_j = \frac{\hat{D}_j}{\hat{D}}$ with:

$$\hat{D}_j = \frac{1}{N}\sum_{k=1}^{N} f(\vec{x}_1^k, ..., \vec{x}_{j-1}^k, \vec{x}_j^k, \vec{x}_{j+1}^k, ..., \vec{x}_{I+L}^k) f(\underline{\vec{x}}_1^k, ..., \underline{\vec{x}}_{j-1}^k, \vec{x}_j^k, \underline{\vec{x}}_{j+1}^k, ..., \underline{\vec{x}}_{I+L}^k) - \hat{f}_0^2,$$

where $(\vec{x}_1^k, ..., \vec{x}_{I+L}^k)_{k=1,N}$ and $(\underline{\vec{x}}_1^k, ..., \underline{\vec{x}}_{I+L}^k)_{k=1,N}$ are two independent sets of N simulations of multidimensional inputs. Like in Sobol method, to evaluate S_j, we change all variables but $\vec{X}_j$.

Second order indices are estimated by the same way, fixing all variables but $\vec{X}_j$ and $\vec{X}_k$ for S_{jk}.

For total sensitivity indices, we use the same method that proposed by Homma and Saltelli [4]. At the inverse of S_j, we fix for S_{T_j} all variables but $\vec{X}_j$:

$$\hat{D}_{\sim j} = \frac{1}{N}\sum_{k=1}^{N} f(\vec{x}_1^k, ..., \vec{x}_{j-1}^k, \vec{x}_j^k, \vec{x}_{j+1}^k, ..., \vec{x}_{I+L}^k) f(\vec{x}_1^k, ..., \vec{x}_{j-1}^k, \underline{\vec{x}}_j^k, \vec{x}_{j+1}^k, ..., \vec{x}_{I+L}^k) - \hat{f}_0^2,$$

and we estimate total index by $S_{T_j} = 1 - \frac{\hat{D}_{\sim j}}{\hat{D}}$.

This method of estimation, like Sobol's for classical sensitivity indices, is very simple and easily comprehensible, but computationally very expensive. It will be interesting to consider LP_τ sequences, like Homma and Saltelli [10].

We illustrate these multidimensional indices with a theoretical application, for which sensitivity indices can be analytically computed.

4.2 Theoretical application

Consider the model $Y = aX_1X_2 + bX_3X_4 + cX_5X_6$, where $X_i \sim \mathcal{N}(0,1)$, for $i =$ 1 to 6, and where X_3 and X_4 are correlated ($\rho_{X_3,X_4} = \rho_1$), as well as X_5 and X_6 ($\rho_{X_5,X_6} = \rho_2$). As X_3 and X_4 are correlated, we consider one multidimensional input (X_3, X_4). Sensitivity index, relative to (X_3, X_4) is noted by $S_{\{3,4\}}$. In the same way, $S_{\{5,6\}}$ expresses sensitivity to input (X_5, X_6). We consider also that this model has 4 independent variables: X_1, X_2, (X_3, X_4) and (X_5, X_6). It is possible to compute analytically value of sensitivity indices. Results are the following:

$$\begin{aligned} S_{12} &= \frac{a^2}{a^2 + b^2(1+{\rho_1}^2) + c^2(1+{\rho_2}^2)}, \\ S_{\{3,4\}} &= \frac{b^2(1+{\rho_1}^2)}{a^2 + b^2(1+{\rho_1}^2) + c^2(1+{\rho_2}^2)}, \\ S_{\{5,6\}} &= \frac{c^2(1+{\rho_2}^2)}{a^2 + b^2(1+{\rho_1}^2) + c^2(1+{\rho_2}^2)}, \end{aligned}$$

and all the other indices are equal to 0.

We note that the value of the numerator of the interaction sensitivity index S_{12} is function of the coefficient a. The values of numerators of the non-zero sensitivity indices $S_{\{3,4\}}$ and $S_{\{5,6\}}$ are function of the model coefficients b and c, but also of the correlation coefficients ρ_1 or ρ_2. We present some numerical values of those indices in Table 1, for different values of the coefficients of the model (a, b and c) and the correlation coefficients.

First of all, let us underline that as X_1 and X_2 are independent variables, indices S_1, S_2, and S_{12} are usual sensitivity indices, and can also be computed without using group sensitivities.

In the situation (i), as X_1 and X_2 are independent variables, usual sensitivity indices allow us to conclude that variance of Y is essentially (73%) due to interaction between X_1 and X_2. But in the others situations where X_1 and X_2 are less important, we need group sensitivity indices to apportion effect to the two couples (X_3, X_4) and (X_5, X_6). These indices allow us to know that the couples (X_3, X_4) and (X_5, X_6) have the same importance in the situation (ii), and that (X_5, X_6) is the most important in situation (iii). Effectively, in situation (ii), the couples (X_3, X_4) and (X_5, X_6) are symmetric in the model, and so they have same importance. In (iii) a coefficient equal to 3 is multiplying the product X_5X_6, the couple (X_5, X_6) is obviously more important than (X_3, X_4).

Situations (iv), (v) and (vi) illustrate that indices $S_{\{3,4\}}$ and $S_{\{5,6\}}$ as well as S_{12} are function to the correlation. As the couples (X_3, X_4) and (X_5, X_6) are in the model in a product form (X_3X_4 and X_5X_6), greater is the correlation, greater is the importance of the couple, and so greater is the value of the sensitivity index. In (iv) the correlation of (X_3, X_4) is greater than the correlation of (X_5, X_6), and so $S_{\{3,4\}}$ is greater than $S_{\{5,6\}}$. In situations (v) and (vi), the same behavior is observed.

This simple application illustrates well the utility of group sensitivity indices when inputs are correlated.

5 Application in nuclear field

This Section presents applications of works presented in Section 3 and 4.

5.1 Impact of model mutation - GASCON radiological impact software

GASCON is a model developed to study the chronological atmospheric releases and dosimetric impact which is used by CEA (French Atomic Energy Commission) for facilities safety assessment. This software evaluates the doses received by a population (called reference group) exposed to the cloud of radionuclides and through the food chains. It takes into account the interactions which exist between humans, plants and animals, the different pathways of transfer (wind, rain, ...), the distance between emission and observation, and the time from emission.

Study [11] presents a sensitivity analysis for this model. The analysis involved:

- uncertainty analysis *via* Monte-Carlo calculations,
- fast sensitivity analysis with correlation coefficients between input and output variables,
- construction of response surfaces requiring negligible computation times,
- calculations of Sobol sensitivity indices.

We focus here on one output of GASCON: Ad_I_1, the annual effective dose in ^{129}I received in one year by an adult who lives in the neighborhood of a particular nuclear facility. We consider the model (7) defined in [11] by the response surface:

$$\begin{aligned} Y = \alpha_0 &+ \alpha_1 X_1 X_2 X_3 X_4 X_5 + \alpha_2 X_1 X_2 X_3 X_4 X_5^2 + \alpha_3 X_1 X_2 X_3 X_6 X_5 \\ &+ \alpha_4 X_1 X_2 X_3 X_6 X_5^2 + \alpha_5 X_1 X_7 X_8 X_9 X_5 + \alpha_6 X_1 X_7 X_8 X_9 X_5^2 \\ &+ \alpha_7 X_1 X_7 X_8 X_{10} X_5, \end{aligned} \tag{7}$$

where Y is the output Ad_I_1, and X_i are the following 10 inputs:

$$\begin{aligned} X_1 &: \text{effective ingestion for an adult}, \\ X_5 &: \text{dry deposit rate}, \\ X_2, X_3, X_4, X_6 &: \text{parameters of goat's milk food chain}, \\ X_7, X_8, X_9, X_{10} &: \text{parameters of ewe's milk food chain}, \end{aligned}$$

and α_i are the regression coefficients presented in Table 2.

Random inputs are bi-uniform on variation interval $[min, max]$, *i.e.* uniform on $[min, nominal]$ with probability $\frac{1}{2}$, and uniform on $[nominal, max]$ with probability $\frac{1}{2}$. The probability density function of such variables is:

$$\rho(x)\begin{cases} \frac{1}{nominal-min}\mathbb{1}_{[min,nominal]}(x) & \text{with} \quad p=\frac{1}{2}, \\ \\ \frac{1}{max-nominal}\mathbb{1}_{[nominal,max]}(x) & \text{with} \quad p=\frac{1}{2}. \end{cases}$$

Table 3 presents values of variation intervals for the 10 inputs, for the nuclear installation studied in [11].

First moments of response surface (7) have been estimated by Monte-Carlo, with 10000 simulations. Confidence intervals have been obtained repeating 200 times this estimation (standard deviation in brackets):

$$\begin{aligned} E[Y] &= 2.0265 \times 10^{-13} \quad (4.5455 \times 10^{-29}), \\ V(Y) &= 3.9544 \times 10^{-25} \quad (1.5093 \times 10^{-51}). \end{aligned} \tag{8}$$

Response surface (7) is used in [11] to compute sensitivity indices (first order and total) by Sobol method. Results are presented in Figure 1.

First application

Assume that, following new information on the model (7), the variable X_1 must be fixed to its nominal value 1.1×10^{-7}. The model thus defined is noted Y'.

Mutation method presented in Section 3 allows us to obtain sensitivity indices of this new model Y', instead of doing a new analysis. Sensitivity indices of Y' can be obtained by multiplying those of Y by:

$$\frac{V(Y)}{V(Y')}\left(\frac{1.1\times 10^{-7}}{E[X_1]}\right)^2. \tag{9}$$

The variance of Y' is estimated by Monte-Carlo simulations, and is equal to $V(Y') \simeq 1.9152\times 10^{-26}$, and so, using Y's moments (8), the coefficient (9) is equal to 2.2564.

Figure 2 presents results thus obtained for sensitivity indices of Y', and results obtained by new analysis. Results are similar, but with mutation method, only an estimation of the variance of the new model is needed. However, for total indices, as they have been estimated directly, *i.e.* without estimating all order sensitivity indices, it is impossible to extract from Y's total indices the interaction of variables with X_1. We need then to estimate total indices by a new analysis.

Second application

Consider the two following models:

$$\begin{aligned} Y_1 = {} & \alpha_1 X_1 X_2 X_3 X_4 X_5 + \alpha_2 X_1 X_2 X_3 X_4 X_5^2 + \alpha_3 X_1 X_2 X_3 X_6 X_5 \\ & + \alpha_4 X_1 X_2 X_3 X_6 X_5^2, \end{aligned}$$

and

$$Y_2 = \alpha_5 X_1 X_7 X_8 X_9 X_5 + \alpha_6 X_1 X_7 X_8 X_9 X_5^2 + \alpha_7 X_1 X_7 X_8 X_{10} X_5.$$

Model Y_1 corresponds to goat's milk food chain and model Y_2 to ewe's milk food chain. Let us assume that the variables X_1 and X_5 are deterministic and fixed to their nominal values (Table 3), such that these two models have no common random variable. Suppose that two sensitivity analyses have been made on these two models. Results of these analyses are presented in Figure 3 and Figure 4.

For the sensitivity analysis of the sum of these two models (which corresponds to model (7), with X_1 and X_5 fixed to their nominal values. It is possible to obtain sensitivity indices of the sum of these two models, by applying mutation method presented in Section 3:

$$S_j = \begin{cases} S_j^1 \times \frac{V(Y_1)}{V(Y_1)+V(Y_2)} & \text{if } j = 2,4,6, \\ \\ S_j^2 \times \frac{V(Y_2)}{V(Y_1)+V(Y_2)} & \text{if } j = 7,8,9,10. \end{cases}$$

Only the variance of the two models Y_1 and Y_2 are needed and have been estimated in preliminary sensitivity analyses:

$$V(Y_1) = 2.2569 \times 10^{-26} \qquad V(Y_2) = 3.814 \times 10^{-28},$$

and so:

$$\frac{V(Y_1)}{V(Y_1)+V(Y_2)} = 0.9834 \qquad \frac{V(Y_2)}{V(Y_1)+V(Y_2)} = 0.0166.$$

Thus, sensitivity indices of $Y = Y_1 + Y_2$ can be computed without performing new simulations and Monte-Carlo estimations. Results are presented in Figure 5 (first order indices) and Figure 6 (total order indices), and are similar to results obtained by a new computationally expensive sensitivity analysis.

The aim of Stay'SL code [12] is to obtain an adjusted neutron spectrum, *i.e.* number of neutrons by energy group, by minimizing the χ^2 value using the following elements:

- measured reaction rates (*i.e.* number of nuclear reaction per second) for each detector; in this study we applied the method on 5 detectors named Det1, Det2, Det3, Det4 and Det5,
- input neutron calculated spectrum,
- nuclear effective cross section issued from nuclear data libraries,
- associated variance-covariance matrix.

This computer code can be seen as a model with 185 inputs and 21 outputs. Input variables are the following:

- $X_1, ..., X_{150}$: 150 efficient sections σ (30 energy groups for each dosimeter Det1, Det2, Det3, Det4 and Det5),
- $X_{151}, ..., X_{180}$: 30 neutron flux Φ (value of the neutron flux by energy group),
- $X_{181}, ..., X_{185}$: 5 reaction rates: τ_{Det1}, τ_{Det2} ,τ_{Det3}, τ_{Det4}, τ_{Det5}.

All these inputs are not independent. Correlation matrix for efficient sections is represented in Figure 7.

In this study, only one output of Stay'SL is considered: Y, the sum of weighted flux of neutrons which have energy superior to 1 MeV.

To apply multidimensional sensitivity analysis using group sensitivities presented in Section 4, the 185 inputs are written into 9 groups of correlated inputs:

- $\vec{X}_1 = (X_1, ..., X_{30})$: nuclear effective cross sections on 30 energy groups for dosimeter Det1,
- $\vec{X}_2 = (X_{31}, ..., X_{60})$: nuclear effective cross sections on 30 energy groups for dosimeter Det2,
- $\vec{X}_3 = (X_{61}, ..., X_{90})$: nuclear effective cross sections on 30 energy groups for dosimeter Det3,
- $\vec{X}_4 = (X_{91}, ..., X_{120})$: nuclear effective cross sections on 30 energy groups for dosimeter Det4,
- $\vec{X}_5 = (X_{121}, ..., X_{150})$: nuclear effective cross sections on 30 energy groups for dosimeter Det5,
- $\vec{X}_6 = (X_{151}, ..., X_{180})$: neutron flux Φ_i given a set of 30 energy groups,
- $\vec{X}_7 = (X_{181}, X_{182})$: reaction rates ($\tau_{Det1}$,$\tau_{Det2}$),
- $\vec{X}_8 = (X_{183}, X_{184})$: reaction rates ($\tau_{Det3}$,$\tau_{Det4}$),
- $\vec{X}_9 = (X_{185})$: reaction rate (τ_{Det5}).

These 9 multidimensional variables are independent.

Group sensitivity indices have been estimated by method presented in Section 4, with 100000 Monte-Carlo simulations. This estimation has been repeated 6 times, to obtain confidence intervals on the sensitivity indices values. Mean and standard deviation for first order and total indices are presented in Figure

8.

The most significant variable is the nuclear effective cross sections for dosimeter Det1, $\vec{X}_1$, with an index approximately equal to 0.5. Then, the second most significant variables are $\vec{X}_4$ and $\vec{X}_7$, nuclear effective cross sections for dosimeter Det4 and reactions rates (τ_{Det1},τ_{Det2}), with indices approximately equal to 0.2. Finally, variable $\vec{X}_6$, neutron flux, and after $\vec{X}_8$, reaction rates (τ_{Det3},τ_{Det4}), have non-null importance but less significant.

It is important to note that the output is not influenced by interactions among the inputs because the sum of first order indices is approximately equal to 1.

6 Conclusion and future work

Two lines of investigation have been described in this paper. The first concerns the computation of sensitivity indices for transformed models for a few tractable cases. Practical applications on a radiological impact software are presented.

In the second, we applied group sensitivities for models with correlated inputs. This work is illustrated by an application in nuclear engineering, on a computer code with a large number of inputs.

Further developments are envisaged, concerning faster estimation of group sensitivity indices. Another application of works on model mutation is the taking into account in sensitivity analysis of the error due to the use of response surface. This application is introduced in [13].

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References

[1] I.M.Sobol. *Sensitivity Estimates for Nonlinear Mathematical Models.* Mathematical Modeling and Computational Experiments, 1993.

[2] M.D.McKay. *Evaluating Prediction uncertainty. Technical Report NUREG/CR-6311.* US Nuclear Regulatory Commission and Los Alamos National Laboratory, 1995.

[3] T.Ishigami, T.Homma. *An importance quantification technique in uncertainty analysis for computer models.* In Proceedings of the ZSUMA '90, University of Maryland, USA, 398-403, 1990.

[4] T.Homma, A.Saltelli. *Importance measures in global sensitivity analysis of non linear models.* Reliability Engineering and System Safety, Vol.52, 1-17, 1996.

[5] A.Saltelli. *Making best use of model evaluations to compute sensitivity indices.* Computer Physics Communications, Vol.145, 280-297, 2002.

[6] R.I.Cukier, H.B.Levine, K.E.Shuler. *Nonlinear Sensitivity Analysis of Multiparameter Model Systems.* Journal of Computational Physics, 1978.

[7] J.H.Schaibly, K.E.Shuler. *Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. II Applications.* Journal Chemical Physics, Vol. 59, 3879-3888, 1973.

[8] A.Saltelli, S.Tarantola, K.Chan. *A Quantitative Model-Independent Method for Global Sensitivity Analysis of Model Output.* Technometrics, Vol.41, No.1, 1999.

[9] A.Saltelli, K.Chan, E.M.Scott. *Sensitivity Analysis.* Wiley, 2000.

[10] T.Homma, A.Saltelli. *Uses of Sobol's Quasirandom Sequence Generator for Integration of Modified Uncertainty Importance Measure.* Journal of Nuclear Science and Technology, Vol.32, 1164-1173, 1995.

[11] B.Iooss, N.Devictor, F.Van Dorpe. *Response surfaces and sensitivity analysis for an environmental model of dose calculations.* In Proceedings of Fourth International Conference on Sensitivity Analysis of Model Output, Santa-Fe (New Mexico-USA), March 8-11, 2004.

[12] F.G.Perey. *Least-Squares Dosimetry Unfolding : The Program STAY'SL.* ORNL/TM-6062 ENDF-254.

[13] N.Devictor, M.Marques, J.Jacques, C.Lavergne. *Advances in methods for uncertainty and sensitivity analysis.* In proceedings of the workshop "Level 2 Probabilistic Safety Assessment", OCDE/AEN/CSNI/WGRISK, Köln (Germany), March, 2004.

FIGURE CAPTIONS

Fig. 1. Sensitivity indices of Ad_I_1 response surface (GASCON).

Fig. 2. First order sensitivity indices of mutated model Y' by mutation ($\times$) and by new analysis ($+$).

Fig. 3. Sensitivity indices of model Y_1.

Fig. 4. Sensitivity indices of model Y_2.

Fig. 5. First order sensitivity indices of model $Y_1 + Y_2$ by mutation ($\times$) and by new analysis ($+$).

Fig. 6. Total sensitivity indices of model $Y_1 + Y_2$ by mutation ($\times$) and by new analysis ($+$).

Fig. 7. Covariance matrix for 150 Stay'SL efficient sections.

Fig. 8. First order and total sensitivity indices of Stay'SL.

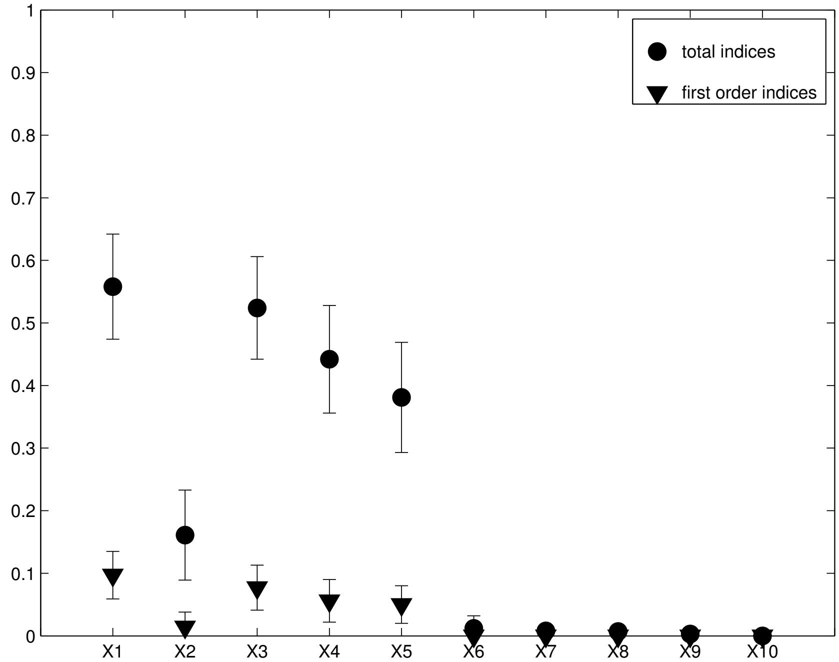

Fig. 1, Jacques et al.

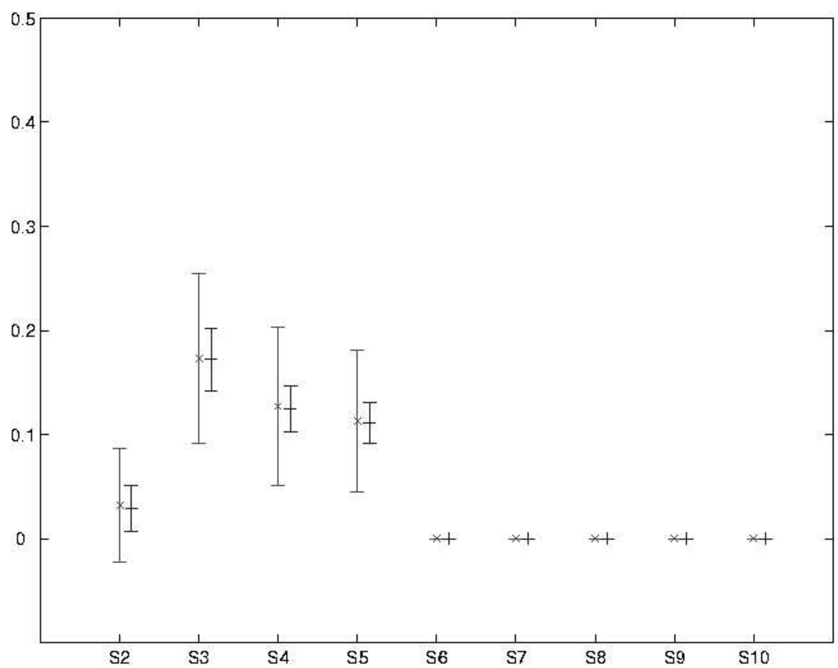

Fig. 2, Jacques et al.

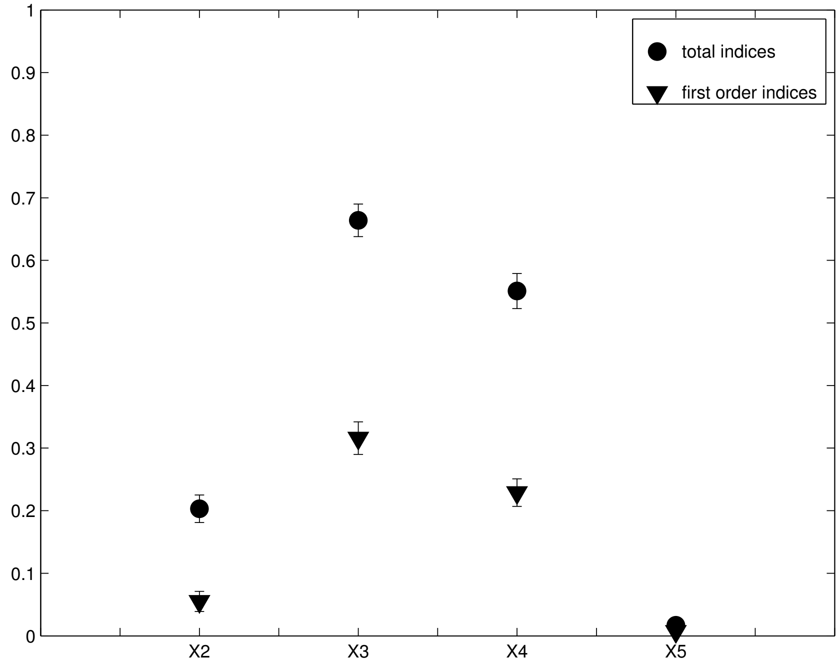

Fig. 3, Jacques et al.

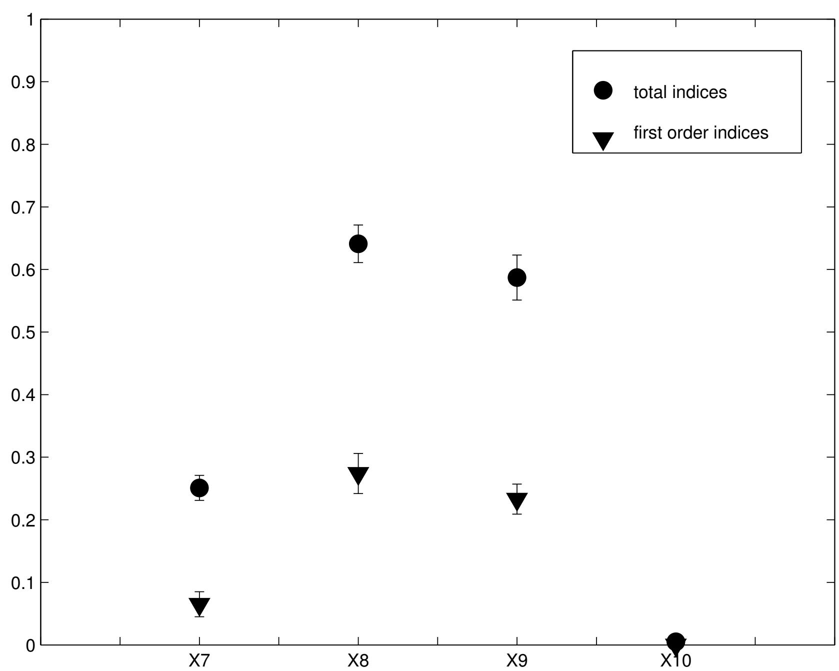

Fig. 4, Jacques et al.

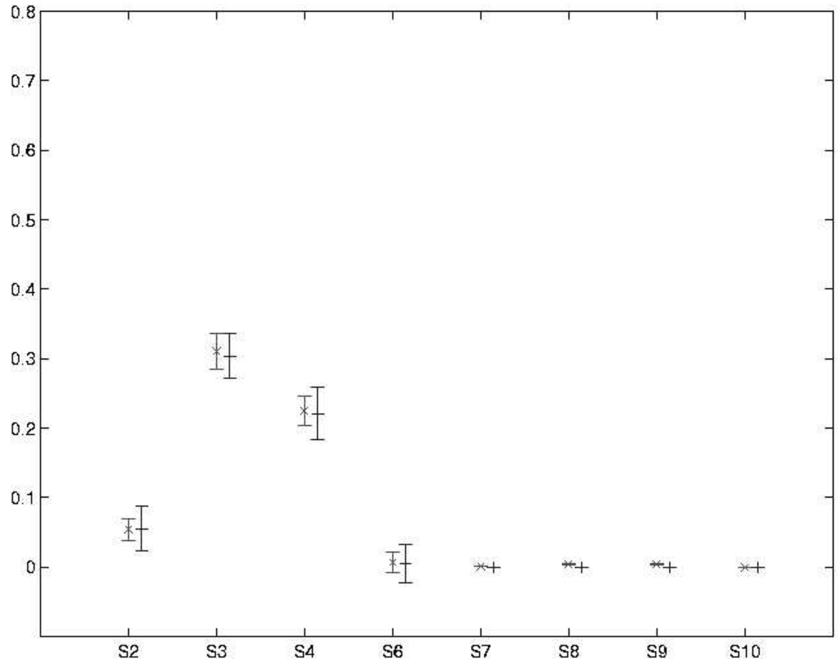

Fig. 5, Jacques et al.

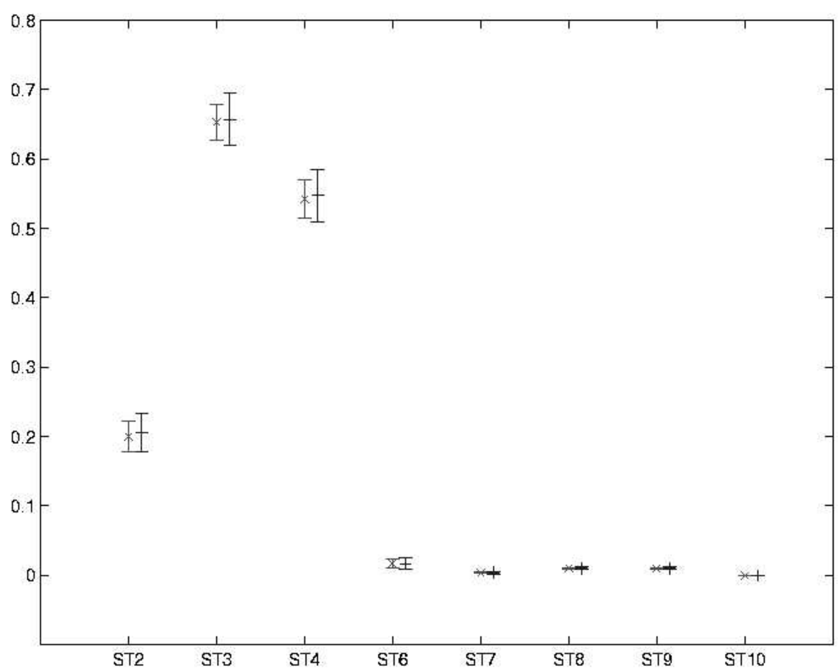

Fig. 6, Jacques et al.

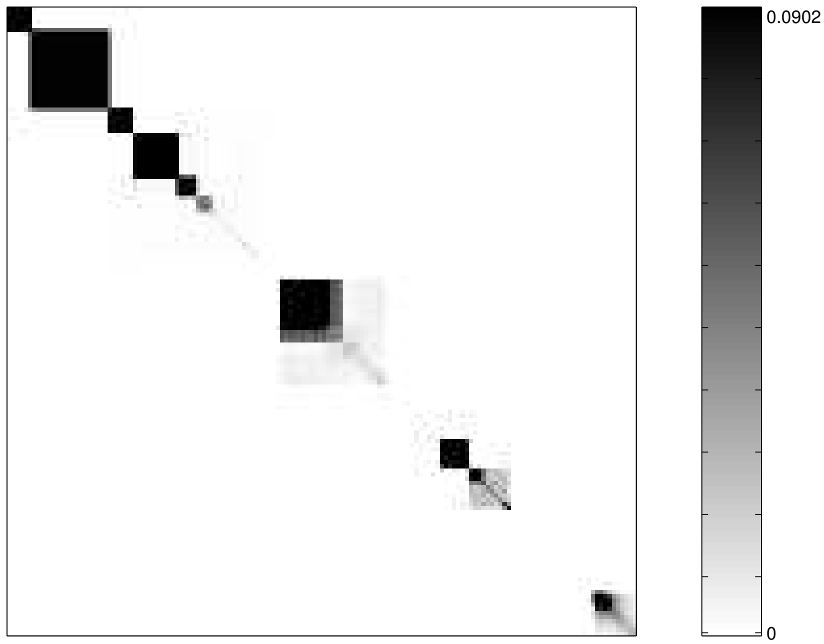

Fig. 7, Jacques et al.

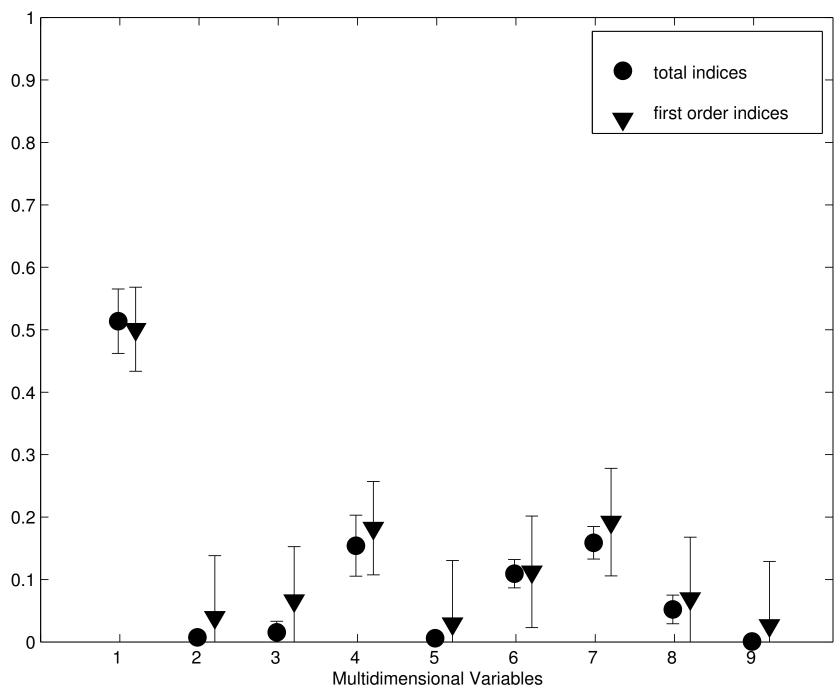

Fig. 8, Jacques et al.

TABLE CAPTIONS

Table 1

Values of sensitivity indices, for different values of the coefficients of theoretical model (a, b and c) and the correlation coefficients.

Table 2

Regression coefficients of Ad_I_1 response surface (GASCON).

Table 3

Inputs variation intervals for Ad_I_1 response surface (GASCON).

situation	a	b	c	ρ_1	ρ_2	S_{12}	$S_{\{3,4\}}$	$S_{\{5,6\}}$
(i)	3	1	1	0.8	0.8	0.7329	0.1336	0.1336
(ii)	1	1	1	0.8	0.8	0.2336	0.3832	0.3832
(iii)	1	1	3	0.8	0.8	0.0575	0.0943	0.8483
(iv)	1	1	1	0.8	0.3	0.2681	0.4397	0.2922
(v)	1	1	3	0.8	0.3	0.0803	0.1317	0.7880
(vi)	1	1	3	0.3	0.8	0.0593	0.0647	0.8760

Table 1, Jacques et al.

coeff.	value	coeff.	value
α_0	1.0303×10^{-14}	α_4	-3.5456×10^{-10}
α_1	5.3945×10^{-11}	α_5	6.2968×10^{-11}
α_2	-8.1069×10^{-10}	α_6	-1.0495×10^{-9}
α_3	2.2303×10^{-11}	α_7	1.0339×10^{-11}

Table 2, Jacques et al.

variable	nominal	min	max	expectation	variance
X_1	1.1×10^{-7}	1.1×10^{-8}	1.1×10^{-6}	3.3275×10^{-7}	1.1536×10^{-13}
X_2	0.43	0.06	0.65	0.3925	0.02947
X_3	110	11	1100	332.75	1.1536×10^{5}
X_4	2557	255.7	25570	7734.925	6.2338×10^{7}
X_5	0.005	0.0005	0.05	0.015125	2.3835×10^{-4}
X_6	1096	109.6	10960	3315.4	1.1452×10^{7}
X_7	0.49	0.08	0.94	0.5	0.06166
X_8	10	1	100	30.25	9.5343×10^{2}
X_9	2557	255.7	25570	7734.925	6.2338×10^{7}
X_{10}	1096	109.6	10960	3315.4	1.1452×10^{7}

Table 3, Jacques et al.