

Response surfaces and sensitivity analyses for an environmental model of dose calculations

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ABSTRACT

A parametric sensitivity analysis is carried out on a radiological impact software describing the radionuclides transfer to the man following a chronic gas release of a nuclear installation. An effective dose received by age group can thus be calculated according to the duration of the release. Due to the large number of input parameters (more than fifty for each output variable) a methodology is proposed. The generation of one thousand Monte-Carlo simulations allows to calculate correlation coefficients between input parameters and output variables, which give a first overview of important factors. Least-squares multiple regression is used to construct response surfaces in polynomial form for each output variable. Then using these polynomials, we calculate the global sensitivity indices of Sobol by the Monte-Carlo method. We show the application of this method to one site of study and to one reference group, for two radionuclides: iodine 129 and uranium 238.

Keywords: Uncertainty, sensitivity analysis, environmental transfer, radiological impact

1. INTRODUCTION

The present study presents the global sensitivity analysis of a radiological impact software called GASCON. GASCON (developed by CEA/DAM/DASE) is dedicated to chronological atmospheric releases and dosimetric impact which is used for CEA facilities safety assessment. This software evaluates the doses received by a population (called reference group) exposed to the cloud of radionuclides and *via* the food chains. It takes into account the interactions which exist between the man, the plant and the animal, the different ways of transfer (wind, rain, ...), the distance between emission and observation, the time passed between emission and calculation, ...

Various stages in the analysis of a process (software, measurement, experiment, ...) introduce potential errors, in particular in the construction of the various models: real phenomenon with the physical model, physical model with the mathematical model, and mathematical model with the numerical model. The principal sources of uncertainties

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are in the approximation made by the modeling of the physical phenomenon, the approximations made on the parameterization of the model, the input data and the input parameters. The uncertainty analysis is used to evaluate the confidence interval or the probability distribution of the result. The global sensitivity analysis is used to quantify the influence of the input parameters uncertainties on the output variables uncertainties. Recent studies have applied different uncertainty analysis and sensitivity analysis methods to environmental models (Helton [6], Campolongo and Saltelli [2], Hedin [5]).

The results provided by GASCON are in the form of annual effective doses (Sv/yr) received by a reference group, divided into three age compartments: adult, child and baby. We also distinguish three operating cycles of the release installation: one year, ten years, fifty years. In our study the reference group is a village near the release installation, and we consider two radionuclides ^{129}I and ^{238}U . There is thus eighteen output variables.

The main ways of exposure taken into account in GASCON are:

- ◇ external exposures: radioactive cloud and soil deposits;
- ◇ internal exposures: inhalation, ingestion of plants contaminated by direct way (foliar transfer by contact with the radioactive cloud) and indirect way (soil deposit then root transfer), ingestion of contaminated animal productions.

Some input data are specific of the studied radionuclide or of the studied site (meteorological conditions, soils nature, feed rations, ...). We have deduced from the literature the variation ranges of parameters considered for the sensitivity analysis, which are:

- ◇ dose factors for external irradiation, effective ingestion, effective inhalation;
- ◇ transfer factors to animal productions (milk, meat of cow, ewe, goat, pig ...);
- ◇ factors of soil-plant transfer (vegetables, cereals, fodder, ...);
- ◇ translocation factors (fruits, vegetables, cereals, ...);
- ◇ sorption coefficients K_d (sands, silts, clays and organic matter);
- ◇ dry deposit rate for each radionuclide;
- ◇ local feed rations of the reference group for the various age compartments (vegetables, fruits, cereals, milk, meat, egg, ...), and animal feed rations (grass, hay, corn) related to the products eaten by the reference group.

The following section presents the four stages of our methodology: 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. In the third section this methodology is applied to the GASCON software using specific nuclear installation and reference group. We discuss the result of this approach and conclude in the last section.

2. METHODOLOGY

2.1. Uncertainty analysis

The general objective of our uncertainty analysis is to evaluate uncertainty on a computation result Y taking into account uncertainties on the input parameters X_i ($i = 1, \dots, N_p$).

It is necessary for each input parameter to evaluate a probability density function (by expert opinion or by a data statistical analysis). The results of the uncertainty analysis is conditioned with the choices of these probability densities. To propagate uncertainties, we use the pure Monte-Carlo strategy: random generation of N samples of input parameters, then software calculation for each sample.

Because of our lack of knowledge, we choose the uniform law for the distribution of all input parameters. Moreover, it requires only the bounds of the parameter variation ranges. However for the majority of the GASCON parameters, an order of magnitude separates the minimal and nominal values ($\min \sim \text{nominal}/10$) and the nominal and maximal values ($\max \sim \text{nominal} \times 10$). Thus, if we choose the uniform function on $[\min; \max]$, the majority of the simulated values will be included in the interval $[\text{nominal}; \max]$. To counter this problem, each simulation proceeds in the following way:

- ★ we simulate a uniform random variable u on $[0; 1]$;
- ★ if $u \leq 0.5$: the simulation value is $2u(\text{nominal} - \min) + \min \in [\min; \text{nominal}]$;
- ★ if $u > 0.5$: the value is $(2u - 1)(\max - \text{nominal}) + \text{nominal} \in]\text{nominal}; \max]$.

From the Monte-Carlo simulations, we obtain for each output variable the elementary statistical parameters (average, minimum, maximum, standard deviation, variation coefficient, skewness and Kurtosis coefficients) and the probability distribution. From the distributions, we can observe the spreading out of the output variables, the confidence intervals, the multiplicity of modes, ... Statistical comparison tests can also be made. In our study, we analyze nine output variables for each radionuclide, and we deduce by the Kolmogorov-Smirnov test (Saporta [11]) which variables are statistically similar.

2.2. Sensitivity analysis with correlation coefficients

The global sensitivity analysis is used to quantify the contribution of each input parameter to the response variability. The linear correlation coefficient ρ (or Pearson coefficient) between two random variables X and Y is the simplest sensitivity index. If ρ is close to $+1$ or -1 , the assumption of linearity between X and Y is valid. If Y is an output variable and if there are several input variables X_j ($j = 1, \dots, N_p$), the correlation coefficients between Y and each X_j have not quantitative sense, but can reveal the linear character of some dominant variables (Saporta [11]).

If the behavior of Y compared to each parameter is overall linear, it is possible to obtain quantitative measurements of their influence from the standard regression coefficients (linear regression connecting Y to the X_j). To obtain a measurement of the linearity of the relation between Y and X_j , we use the partial coefficients of correlation p_j . In opposition to the standard regression coefficients, the partial correlation coefficients allow to eliminate the influence from the other variables (Saltelli et al. [9]). If the relation between X and Y is not linear, the correlation coefficients of the ranks (or Spearman coefficients) can be used. By replacing the values of parameters X^1, \dots, X^N and of output variable Y^1, \dots, Y^N by their rank, the assumption of linearity is thus replaced by the assumption of a monotonous relation.

The regression or correlation coefficients are related to linear or monotonous assumptions. Moreover, they study only the relations between the output variable and an input

parameter independently of the other parameters. However, many problems are neither linear nor monotonous, and reveal physical dependences between parameters. Global sensitivity analyses more adapted to these conditions are available, but they are definitely more expensive in computing times (Saltelli et al. [9]). In order to test them on GASCON, it is necessary to simplify this software and to replace it by a response surface.

2.3. The response surface method

The response surface method (Box and Draper [1], Kleijnen [8]) is used to build a function which simulates the behavior of a physical or chemical phenomenon in the field of variation of the influential parameters, starting from a certain number of experiments. In our study, an experiment is a calculation by the GASCON software. Building a response surface (RS) aims to obtain a mathematical model representative of the studied software, having good capacities of prediction, and whose computing time to evaluate an output variable is negligible. Such a RS will be thus effective for the uncertainty and sensitivity analyses, requiring several thousands of simulations.

To build a RS, it is necessary to have the software H which models the studied phenomenon, a sample D of N points $(\mathbf{x}(i), z(i))$, where $\mathbf{x}(i)$ is a vector of the N_p random input parameters and $z(i) = H[\mathbf{x}(i)]$ ($i = 1 \dots N$) is the software response, and a family F of functions $f(\mathbf{x}, \mathbf{c})$, where \mathbf{c} is a vector of parameters (parametric regression) or indices (nonparametric regression) which makes possible the identification of the various elements of F . There are multiple RS families (Hastie et al. [4]): polynomials, interpolating radial functions, splines, generalized linear models, partial least squares, neural networks, support vector machines, ... In this work, we use only polynomials, because they have a simple physical interpretation and the majority of the GASCON equations are linear formulas compared to each variable.

In general, we use the technique of least squares to obtain the best representing f_0 in the family F . We minimize the function $\sum_{i=1}^N \{z(i) - f[\mathbf{x}(i), \mathbf{c}]\}^2$ in relation to the parameters \mathbf{c} , to obtain \mathbf{c}_0 and the RS $f_0(\mathbf{x}) = f(\mathbf{x}, \mathbf{c}_0)$. The RS quality of approximation is given from a statistical analysis on a construction basis, whereas the quality of prediction is deduced from a prediction basis. A simple method to qualify a RS is to compare on the two bases some indicators obtained from the RS with those obtained directly with software H . In our study, we initially compare their average, standard deviation, minimum and maximum. In addition, a regression analysis allows to determine the share of variability of the output variable explained by the model. Other possibilities to validate RS are the cross-validation or bootstrap techniques (Hastie et al. [4]). For simplicity, we just present two statistics which give global measurements of correlation between two data sets A and B : the Pearson correlation coefficient ρ and the coefficient of determination R^2 which writes

$$R^2(A, B) = 1 - \frac{\sum_{i=1}^N (A_i - B_i)^2}{\sum_{i=1}^N (\bar{A} - A_i)^2}, \quad (1)$$

where \bar{A} is the average of A . The coefficient R^2 represents the fraction of the variation compared to the average explained by the smoothed model, i.e. the percentage of output variables explained by the response surface. In our case, A is the software response $A_i = z(i) = H[\mathbf{x}(i)]$ and B is the model (RS) response $B_i = f[\mathbf{x}(i), \mathbf{c}_0]$.

These criteria are global and it is possible that the data adjusted are not homogeneous. It is the case when the studied variable covers a broad range of variations with multiple orders of magnitude. In this case, the contributions of the low values to the R^2 measurement are negligible. To cure this problem, the study of residual statistics gives some indications of the regression accuracy. The residuals ϵ have to be centered with a standard deviation σ_ϵ small compared to the GASCON standard deviation σ_A . We also examine the average and the standard deviation of the relative residuals $\epsilon_i/B_i = (A_i - B_i)/B_i$.

2.4. Global sensitivity analysis

We consider methods of variance analysis which aim at determining the weight of the variance of the response $Y = f(X)$ resulting from a variable or a group of variables (McKay [7], Saltelli et al. [9]). Their objective is to calculate the global sensitivity index St_i defined as the sum of all the sensitivity indices implying parameter X_i . The Sobol method allows a relatively simple evaluation of the terms S_i, S_{ij}, \dots (Saltelli et al. [9]).

In practice, we can evaluate Sobol indices by a Monte-Carlo method, which require a very significant number of simulations, typically $N_s = 10000$ to estimate an index of a parameter (S_i, S_{ij}, \dots or St_i). This justifies the use of response surfaces to minimize the computing times. Although the calculation of Sobol index with FAST method is definitely less expensive, we use the Monte-Carlo method because we obtain a realistic confidence interval on the Sobol index by repeating the index calculation. This information is essential if we want to rigorously classify the influence of the various input variables. In our study, we carry out $N_{ic} = 200$ calculations of each Sobol index. Moreover, the Monte-Carlo method calculates all the Sobol indices (S_i, S_{ij}, \dots or St_i), which bring information on the interactions between the input parameters. In our study, we just calculate S_i and St_i to measure the influence that the variable X_i has while acting alone. The Monte-Carlo method calculates these two indices using the same N_s simulations (Saltelli [10]), whereas FAST calculates them starting from two different sets of simulations.

For the model $Y = f(X)$ where X is a vector of N_p parameters, we need $N_{ic} \times N_s \times (N_p + 2)$ evaluations of f to calculate the first order indices S_i and total indices St_i for all the parameters X_i , and to allocate a confidence interval to them. In our study, $N_s = 10000$ and $N_{ic} = 200$. The value of N_p depends on the model of response surface which is adjusted. For GASCON, we try to take into account no more than ten parameters in each response surface. For $N_p = 10$, there will be 2.4×10^7 calculations of f .

3. RESULTS

The GASCON software is applied to a French nuclear research center. The gas release is fixed at a symbolic value of 1 Bq/year which does not represent a realistic release. This also induces non realistic effective dose rates. We perform one thousand independent Monte-Carlo simulations of the GASCON software (30 seconds per simulation). In Figure 1, the distributions of the 18 output variables are represented. For a given radionuclide, the output variable distributions seem very similar. We carry out statistical tests between the coherent output variables (same radionuclide, same age compartment or same operating cycle) by the Kolmogorov-Smirnov test which evaluates if there are or not statistically

significant differences between the two distributions on the degree of confidence 95%. For ^{129}I , there is no difference at 95% between all the distribution couples, except between (adult, operating cycle of 50 years)/(baby, operating cycle of 1 year) and (adult, operating cycle of 50 years)/(baby, operating cycle of 10 years). For ^{238}U , all distribution couples have differences at 95%, except for (adult, 1)/(adult, 10), (child, 1)/(child, 10), (baby, 1)/(baby, 10). In summary, the variables at ten years have approximately the same distributions than the variables at one year, and for ^{129}I the variables "child" have the same distributions than the variables "adult". Thus for ^{129}I and ^{238}U , it is sufficient to study four output variables: (adult, 1), (adult, 50), (baby, 1), (adult, 50).

Table 1 shows the largest Pearson and Spearman correlation coefficients between input and output variables. All the output variables reveal five important input parameters: the dose factor of effective ingestion *ingeff*, the human feed ration of goat's milk *ra_gmilk*, the goat feed ration of grass *ra_grass*, the dry deposit rate *dep*, and the transfer factor to the goat's milk *gmilk*. For ^{238}U , some additional parameters appear: the goat feed ration of cereals *ra_cer* and the transfer factor of the vegetables fruits *vegfr*.

ρ ρ^S	<i>ingeff</i>	<i>gmilk</i>	<i>ra_gmilk</i>	<i>ra_grass</i>	<i>dep</i>	<i>ra_cer</i>	<i>vegfr</i>
Ad_I_1	33 55	09 16	31 46	28 41	21 38		
Ad_I_50	33 56	09 16	31 45	28 41	21 39		
Bb_I_1	32 54	09 16	31 47	28 42	21 37		
Bb_I_50	32 54	09 16	31 47	28 42	21 38		
Ad_U_1	28 55	20 24	21 29	18 26	15 20	08 11	
Ad_U_50	36 62	17 19	18 21	15 20	20 29		10 19
Bb_U_1	25 53	21 33	21 37	18 33	15 26	08 10	
Bb_U_50	27 59	20 29	21 32	18 28	16 21	08 08	

Table 1. Correlation coefficients (in %) of Pearson ρ and Spearman ρ^S between the output and input variables (selected if ρ and ρ^S are higher than 8%). The notation Ad_I.1 means (adult, ^{129}I , one year of release).

At present, for each output variable, we want adjust a response surface by a polynomial model obtained by multiple regression. By selecting and combining the parameters found in Table 1, the best results are obtained when the regressions are made according to certain food chains, which are linear combinations of the various terms contributing in each chain. For example, the food chain of the goat's milk is

$$\alpha_1 * ingeff * gmilk * ra_gmilk * ra_grass * dep + \alpha_2 * ingeff * gmilk * ra_gmilk * ra_grass * dep^2 + \alpha_3 * ingeff * gmilk * ra_gmilk * ra_hay * dep + \alpha_4 * ingeff * gmilk * ra_gmilk * ra_hay * dep^2, \text{ where } \alpha_i \text{ (} i = 1, \dots, 4 \text{) are regression coefficients.}$$

For all the output variables in ^{129}I and for the variables (^{238}U , baby, 1) and (^{238}U , baby, 50), the response surfaces are polynomials based on the food chains of the goat's milk and the ewe's milk (the same than the goat's milk by replacing the goat by the ewe). For the variables (^{238}U , adult, 1) and (^{238}U , adult, 50), response surfaces include also the effective inhalation term $\alpha_1 * inheff$. For (^{238}U , adult, 50), we add the food chain of the pig's meat and the food chain of the vegetable fruits by indirect transfer:

$$\alpha_1 * ingeff * vegfr * ra_vegfr * dep + \alpha_2 * ingeff * vegfr * ra_vegfr * dep^2.$$

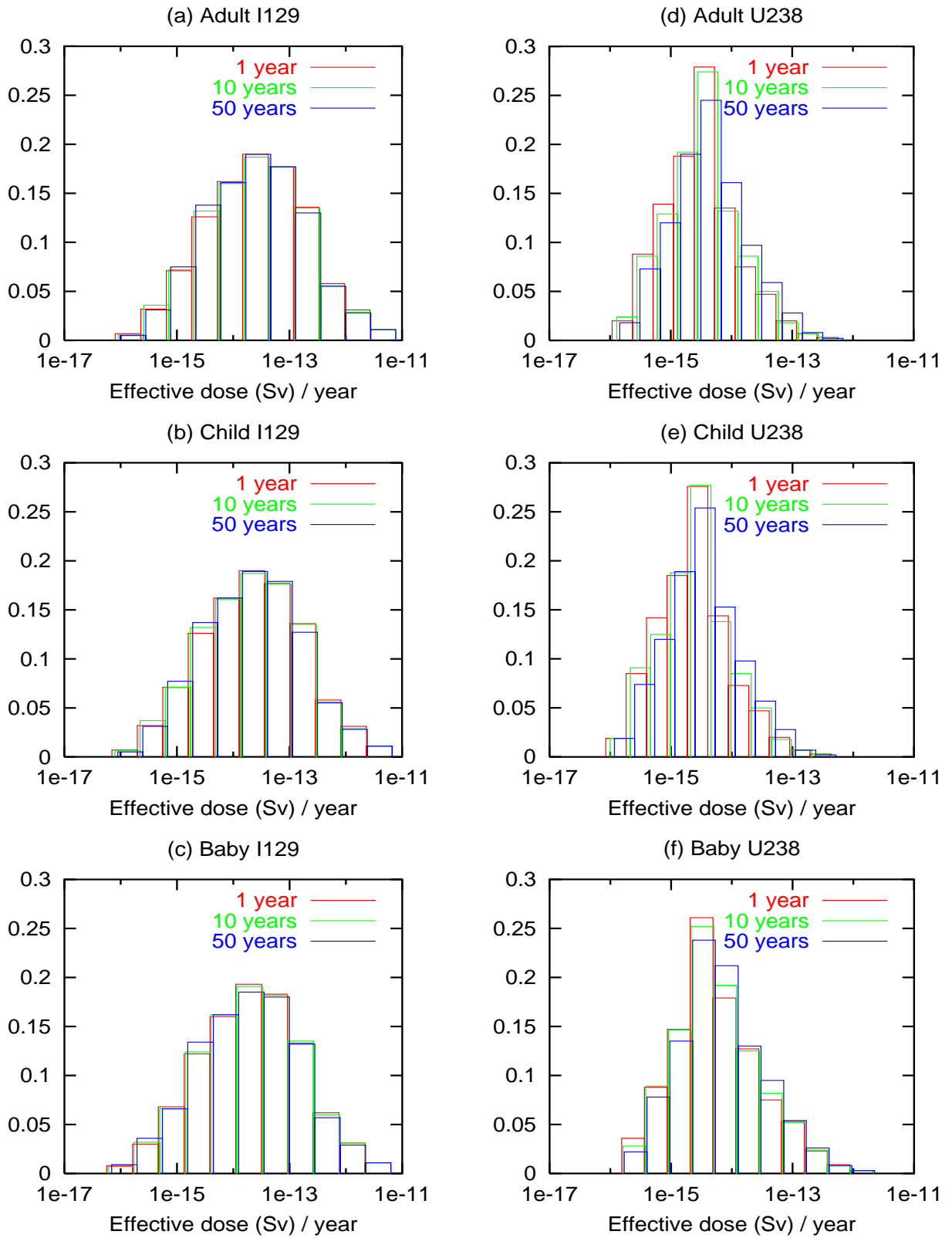


Figure 1. Output variable distributions (Sv/year).

The statistical validity of the RS is studied on a basis of construction (of size 2/3 of the data base) and on a basis of prediction (of size 1/3 of the complete data base). For ^{129}I , the statistics of the R^2 and ρ are excellent: they are equal to 99% for all the variables and on the two bases. The responses in ^{129}I of the GASCON software are almost entirely explained by the terms of the food chain of the goat's milk. For ^{238}U , the statistics R^2 and ρ are also satisfactory (all higher than 92%). It is necessary to integrate in the model the food chains of the goat's milk, the ewe's milk, the effective inhalation, and the pig's meat. In addition, at fifty years, the food chains of vegetables by indirect transfer seem essential. It is noticed that the dry deposit rate dep operates linearly and quadratically in the food chains. This is due to the fact that the relations in GASCON utilize dep like a power of another factor.

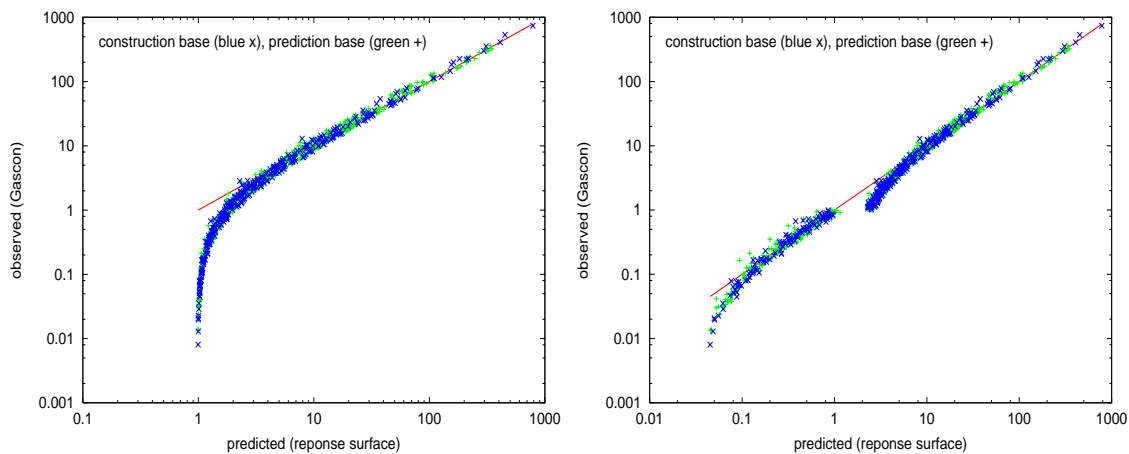


Figure 2. For the adult, ^{129}I and one year of release, comparisons between response surface and GASCON calculations for the two bases (construction and prediction). Unities have to be multiplied by 10^{-14} Sv/year.

It thus seems that the RS are valid but the relative statistics balance our judgement: the relative standard deviations σ_ϵ/σ_A are worth roughly 10% for ^{129}I and 20% for ^{238}U . This lets suppose that the adjustments are not good everywhere. The calculation of the averages and standard deviations of the relative residuals confirms this judgement. For ^{129}I , the representativeness of GASCON by the RS is on average of -30% . For ^{238}U , the representativeness of GASCON by the RS is on average of -15% . The Figure 2 (left) makes it possible to locate the problem thanks to a comparison on the Ad_I_1 variable between GASCON and RS in logarithmic scale. It is noted that the high values ($> 10^{-14}$ Sv/yr) are well adjusted, whereas the low values are completely over-estimated by the RS. To cure this, we propose to separate the construction and prediction bases in two parts each one (one with values higher than 10^{-14} Sv/yr and the other with values lower than 10^{-14} Sv/yr). We choose the same factors of regression for the calculation of the RS. The adjustments are presented in Figure 2 (right). The two RS correctly explain the data in each field of variation with the same factors of regression. This is confirmed by the averages and standard deviation of the relative residuals on the basis of construction which are equal to -13.7% and 22.2% for the raised values, and -4.6% and 22.2% for the

low values, instead of -28.6% and 36.2% on all the variation domain. This problem of regression on a field of several orders of magnitude can be solved in a more satisfactory manner by using the technique of weighted least squares. In the minimization of the functional, we allocate larger weights to low values. This makes it possible to have a homogeneous response surface on all the field of variation.

Now, the GASCON software can be replaced by the RS (polynomial model) which can be used to calculate Sobol indices by extensive Monte-Carlo computations. Figure 3 gives for each output variable the Sobol indices of the most influential variables, with their error bars. Having repeated 200 times the Sobol calculations, the average values are good estimates of the true Sobol indices. We conclude that for ^{129}I , the most influential parameters are the dose factor of effective ingestion and the feed ration of the goat's milk. For ^{238}U , the most influential parameters are the dose factor of effective ingestion, the transfer factor of the goat's milk and the feed ration of the goat's milk.

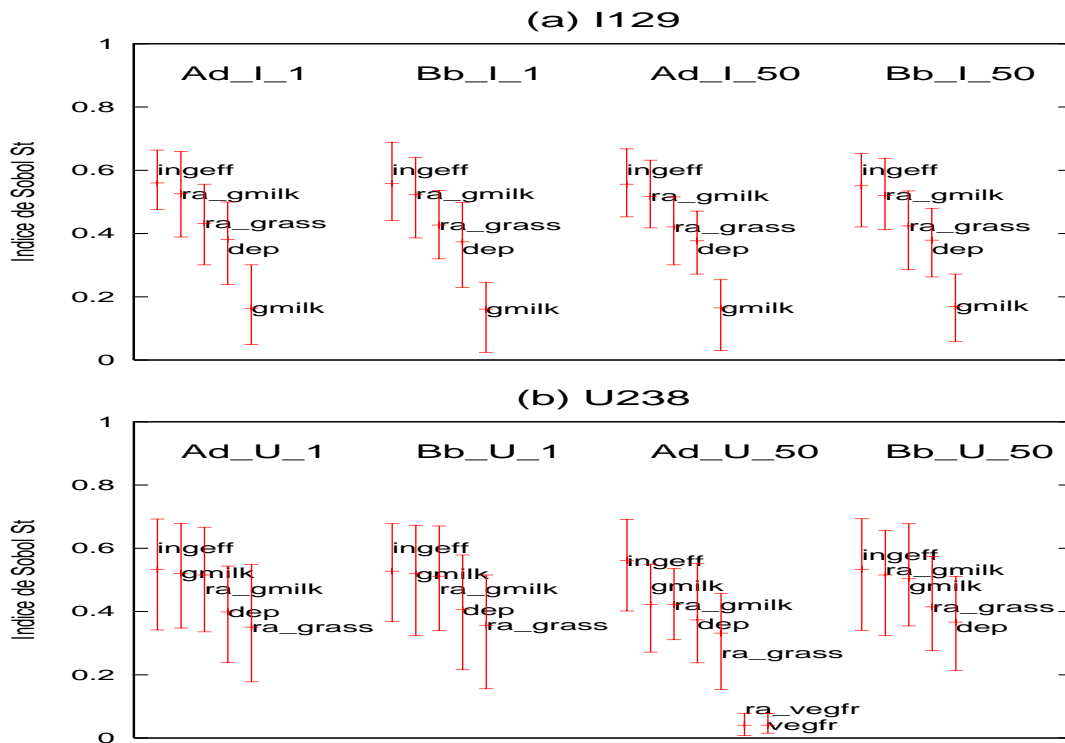


Figure 3. Sobol indices for each parameter. Uncertainty bar represents the minimum, average and maximum indices obtained with 200 Sobol calculations.

By carrying out calculations of the Sobol indices on the RS obtained by distinguishing high values ($> 10^{-14}$ Sv/yr) and low values ($< 10^{-14}$ Sv/yr), we find exactly the same results in the field of high values. In the field of low values, the classification is similar except that the dry deposit rate is placed in first position at equality with effective ingestion. It is thus considered that our results are valid in the field of the high values and are approximately correct in the field of the low values.

4. CONCLUSION

The four steps of our methodology (Monte-Carlo simulation, correlation coefficients analysis, response surfaces, Sobol indices) have allowed to quantify the influence of input parameters on the GASCON software response (annual effective dose received by the man), for a specific nuclear installation, a specific population, and for two radionuclides (^{129}I and ^{238}U). During the correlation coefficient analysis, the calculations of standard regression coefficients would allow to have more information on important input parameters. During the response surface construction, other statistical validation methods like cross-validation or bootstrap technique could also be useful (Hastie et al. [4]). In this work, the response surfaces found are in simple polynomial form explicit for the physicist understanding. For the approximation of software simulating more complex phenomena, more elaborated and not explicit response surfaces, like neural networks (Devictor and Martinez [3]), can be used.

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