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Convergence of sensitivity analysis methods for evaluating combined influences of model inputs

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Abstract

This work aims at studying Morris' extension method to evaluate the contribution of combined variations of inputs to variations of a model output. There is a lack of studies on the Morris' extension method concerning crucial choices of the adequate number of trajectories to distinguish influential and non-influential groups of pairs of inputs, rank pairs of inputs according to their relative importance and reach out the stability of sensitivity indices values. The Morris' extension method was studied regarding the three previous issues via applications on simple and complex models, in comparison with total interaction indices of Sobol. Formal criteria were implemented to assess the convergence of sensitivity analysis results. Sensitivity indices based on the median of mixed elementary effects (MEE) were investigated and found to be competing with classical ones based on the mean of MEE, to achieve convergent results.

Keywords: sensitivity analysis; combined action; Morris' extension method; Sobol method; carbonation model.

1. Introduction

Sensitivity analysis (SA) methods are valuable tools to study how uncertainty about the output of a model can be attributed to different sources at the input of the model [1-3]. SA has been developed in the literature with many proposed improvements, offering different solutions depending on the objective. These methods can be used to verify a model, to understand the mechanisms (individual influences and interactions) within a model, to simplify a model or determine the priority of input parameters. Thus, the SA methods are helpful to provide guidance on the reliability of a model and its predictions. Indeed, many models representing various types of systems (e.g., biological, agricultural, civil engineering) are considered as being “complex” due to both the large numbers of input parameters and non-negligible potential interactions between these inputs that affect response variables [4]. For most of complex models, relationships of the interacting parameters are not precisely known. For instance, the model response is different when two or more inputs vary simultaneously in comparison with the case where inputs vary successively one after the other.

Main goals of SA studies are to define and characterize the influence of individual (or pairs, triplet, etc.) input parameters on the model response [5, 6]. This includes (i) identifying the influential and non-influential inputs, i.e. whether the input parameters have or do not have a significant contribution one another to the variation of the model output; (ii) quantifying relative importance of inputs, i.e. the amount of variation of the response caused by variation of one input relatively to other input parameters; and (iii) identifying the type of their influence, i.e. linear or not, monotonic or not, and their sense, i.e. decreasing or not.

To address these issues, various SA methods are available in the literature. One group of methods is considered as local SA methods, which measured the output sensitivity to the variations of the inputs from their nominal values one at a time (OAT). Local SA used a sampling strategy in which output variations are calculated by varying one input parameter at a time, while keeping all others constant [7]. Another group of methods is considered as global SA methods, which are characterized by the exploration of the entire space of the input parameters. This includes Morris elementary effects method [8] using OAT sampling strategy and its extension for the case of mixed effects [9, 10], methods based on linear regression (standard regression coefficient, linear regression coefficient and partial correlation coefficient) [11], those based on the derivatives [12, 13] (derivative-based global sensitivity measures, DGSM [14] and crossed-DGSM [15]) and on the moment independent (PDF and CDF based) [5, 16, 17], and the methods based on the decomposition of the variance (Sobol indices) [18, 19]. These methods are particularly valuable tools for the development, analysis, and use of

computer models, although the most have generally a high computational cost [7]. However, the Morris methods provide valuable information at low computational cost, making them suitable tools to use for complex models. These methods are a global extension of local perturbation approach within the input parameter space. Reviews of different types of SA methods are available in the literature [1]. A comparison of main SA methods based on certain characteristics is provided in **Table 1**.

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SA Methods	Type				Order of calculated sensitivity indices					Identifying the sense of influence		Identifying the shape of influence						Calculation cost (number of model evaluations)
												Individual influence				2 nd order interaction influence		
	Local	Global	Qualitative	Quantitative	First order	Total influence	Second-order interaction	Higher-order interaction (order > 2)	Total interaction	Individual influence	Interaction influence	Linear	Non-linear	Monotonic	Non-monotonic	Bilinear	Non-bilinear	
OAT [7]	✓	✗	✓	✗	✓	✗	-	-	-	-	-	✗	✗	✗	✗	-	-	$n \cdot (2n + 1)$
Morris [8]	✗	✓	✓	✓	✗	✓	✗	✗	✗	✓	✗	✓	✗	✗	✗	-	-	$r \cdot (n + 1)$
Morris' extension [9, 10]	✗	✓	✓	✓	✗	✗	✗	✗	✓	✗	✓	✗	✗	✗	✗	✓	✗	$r \cdot (n^2 - n + 2)$
Indices based on linear regression (SRC, PCC) [11]	✗	✓	✗	✓	✓	✗	-	-	-	-	-	✓	✗	✗	✗	-	-	$N \cdot n$
Indices based on the derivatives (DGSM and crossed-DGSM) [14, 15]	✗	✓	✗	✓	✗	✓	✗	✗	✓	✗	✗	✗	✗	✗	✗	✗	✗	$N \cdot (n + 1)$
Sobol [18]	✗	✓	✗	✓	✓	✓	✓	✓	✓	✗	✗	✗	✗	✗	✗	✗	✗	$N \cdot (n + 2)$
Moment independent (PDF & CDF based) [5, 16, 17]	✗	✓	✗	✓	✓	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	$N + n \cdot (N \times N)$

Notations: (✓) means that the characteristic is obtained by the SA method, (✗) means that the characteristic is not obtained or difficult to interpret by the SA method and (-) means that the characteristic is not considered or not suitable. n =number of input parameters; N = sample size (~ 10000 for Sobol [20] and ~ 100 to 1000 for indices based on the derivatives, DGSM [21]); r =number of replications or number of trajectories used for Morris and Morris' extension method (~ 10 to 50 for Morris method [22] and more for Morris' extension, depending on the complexity degree of model).

Table 1: Comparison between SA methods according to various characteristics of calculation costs and obtained information

All characteristics are essential to choosing a suitable SA method depending on the objectives, and the choice must be based on the principles of each method and its calculated indices. First, the type of method may depend on the calculation of SA indices. These indices are computed using a local variation by calculating the output model variations with respect to each input parameter or global variation that is characterized by the exploration of input parameters space. Second, the method's type may also depend on the type of the resulting

information from these indices, whether qualitative or quantitative results. For example, Morris and Morris' extension methods produce a qualitative classification order of the input parameters according to their relative importance on the model output and normalized indices that can be considered as semi-quantitative measures to quantify the influence of inputs, while Sobol method allows us to quantify these influences. Third, SA methods differ by the ability of their indices to analyze first order, second order or higher order (combined-actions) sensitivities. Fourth, some SA methods allow identifying the influence sense of individual and interaction effects. This requires that calculation of indices include the sense of variations of model output according to the senses of variations of input parameters. This is the case for the mean of elementary effects (EE) or mixed elementary effects (MEE) in Morris and Morris' extension methods. Fifth, some SA methods can also provide information on the model shape when the analytical equations are not known (i.e. numerical models). These characteristics depend on the calculated sensitivity indices. For example, for Morris' method, a small value of the standard deviation of EE indicates a linear or quasi-linear relationship between the output and the individual input parameter. On the contrary, a high value of the standard deviation of EE indicates either a non-linear, a non-monotonic or an interaction effect [23]. Likewise, for Morris' extension method, small and high values of the standard deviation of MEE respectively indicate a bilinear or quasi-bilinear relationship and a non-bilinear or non-monotonic relationship between the input pairs and the output [10]. Finally, the calculation cost (i.e. the total number of model evaluations N_{ev}) of methods depends on the number of input parameters (n), the number of trajectories (r) and the sample size (N) used in the sampling strategy to calculate sensitivity indices.

SA is frequently required as a method to identify and characterize the relationships of interacting factors, and their influence on a model response is a crucial issue in many studies. For instance, in human genetics, the identification of risk loci and their interactions investigated [24]. Likewise, in medicine, a SA technique is developed for interaction analyses between biological and chemical exposures, which is a challenge in epidemiologic research and can bias effect measures [25]. In building energy models, the relative influence of a couple of input parameters is investigated for developing models that take into account coupling between phenomena, such as occupancy, micro-climate and building envelope [23, 26]. Particularly, in the latter study, the Morris' extension method is applied to identify the most influential pairs of inputs.

Morris' extension method and the total interaction Sobol indices are efficient to detect (screening) and to prioritize (ranking) influential pairs of inputs, and they both provide complementary information. On one hand, the Morris' extension method has an acceptable calculation cost (number of model evaluations) in the screening and ranking of the influential pairs of inputs relative to combined-action influence on the model output, and can identify the sense of the combined-action influence (**Table 1**). On the other hand, the total interaction Sobol indices are useful to determine the total contribution of the combined-actions influences to the variability of model response for all possible pairs of inputs, but its calculation cost is high (**Table 1**). To obtain the total interaction of the combined-actions influences and reduce the calculation cost, as previously proposed for the individual input effects [27-29], one could apply the Sobol method to the most influential pairs (i.e. reduce the number of considered parameters n in **Table 1**), those being previously selected among the most influential ones at lower calculation cost from the Morris' extension method.

However, in studies that used Morris' extension method, e.g. [23, 26], (i) there is a lack of issues concerning stability and convergence of results and (ii) the sensitivity indices are essentially based on calculation of mean of mixed elementary effects (MEE), relative to two or more inputs. The choice of the "optimal" number of model evaluations and sample size that is sufficient to provide convergent results is a critical step of SA methods. The total number of model evaluations in SA methods varies according to the number of input factors and the complexity of the model. Studies in the literature suggest choices for number of evaluations and sample size [30, 31]. Recently, a more rigorous study was conducted for assessment of convergence of SA methods [32]. However, this study only focused on first order analysis and there is thus a lack of knowledge on the convergence of second and higher order analysis. Moreover, the sensitivity indices based on the median of MEE are less frequently studied than those based on the arithmetic mean. Nevertheless, the median is a descriptive statistic that may be more informative about the order of magnitude of variables than the mean, which aggregates the information concerning the repartition of a variable.

This work is a contribution to the assessment of three types of convergence of the Morris' extension screening method and total interaction Sobol index: (i) convergence of screening to distinguish influential and non-influential pairs of input parameters, (ii) convergence of ranking to order the pairs of input parameters according to their contribution to output variance, (iii) convergence of the sensitivity indices values. In addition, the convergences of screening and ranking results of the Morris' extension method are particularly investigated according to indices based on the median of MEE, in comparison to the classical

indices based on the mean of MEE. Formal criteria are presented to assess the convergence of sensitivity analysis results for pairs of input parameters, adapted from the case of individual input parameters [32]. The convergence of results of the SA methods is illustrated on a theoretical model having simple (bilinear) effects and a more complex model from civil engineering having non-linear effects. The first model is a theoretical model defined on the four-dimensional cube [9] which is a simple model and the second is a complex model from civil engineering [33]. Moreover, the robustness of methods is analyzed, via the number of trajectories and the number of simulations, to obtain convergent results depending on the type of model. Note that this work is interested in the influence of interacting input parameters on model output that means if we act on these two inputs at the same time, the result of the model output changes.

This paper is organized as follows. Section 2 presents the Morris' extension method and Sobol indices to identify the influence of combined-action of two input parameters on model output. Section 0 illustrates methods performance on two models chosen through simulations. Section 2 contains discussions of the results. Finally, some concluding remarks are given in Section 5.

Nomenclature abbreviations, symbols and nomenclature

μ	Mean of elementary effects
μ^*	Mean of absolute values of elementary effects
σ	Standard deviation of elementary effects
γ	Median of elementary effects
γ^*	Median of absolute values of elementary effects
E_i	Simple elementary effect
EE_{ij}	Second order elementary effect
dd_{ij}	Mixed elementary effect (MEE)
S	Sobol index

Variables, parameters and indices

RH	Relative external humidity
T	Ambient temperature
CO ₂	CO ₂ -concentration in the air
C	Cement content
W/C	Water to cement ratio
S/G	Sand to gravel ratio
S_max	Maximum nominal aggregate size
CEM	Cement type
f_{cem}	Cement compressive strength
d	Concrete cover depth
t_c	Initial curing period
t_{ser}	Service life
V	Variance
X	Vector of input parameters of a model
Y	Model output variable

2. Sensitivity analysis methods

This section presents first the Morris' extension method [9] then the Sobol indices [18]. Henceforth, we consider a mathematical model which, to a set of random independent input parameters $X = (X_1, \dots, X_n)$, maps a random output variable (or response) Y via a deterministic function f :

$$f : \mathbb{R}^n \rightarrow \mathbb{R}$$

$$X \mapsto Y = f(X)$$

2.1. Morris' extension method [9]

This method aims at studying the influence of combined-actions of two input parameters on model output, while maintaining good computational efficiency. Similarly to Morris' approach to the calculation of simple EE (recalled in **Section I** of Supplementary material), experimental designs are presented to allow the detection of MEE (i.e. related to two or more input parameters) when performing a preliminary screening of model inputs with n input parameters. The Morris' extension method plays the role of screening for combined-actions of model inputs [9].

For a given value x of the input vector of the input parameter space $Q_n \subseteq \mathbb{R}^n$, the double (second in the nomenclature) elementary effect EE_{ij} ($1 \leq i \leq j \leq n$) attributable to the pair of the input parameters (X_i, X_j) is defined as:

$$EE_{ij}(x) = \frac{f(x + e_i \Delta_i + e_j \Delta_j) - f(x)}{\Delta_i \Delta_j} \quad (1)$$

where $\Delta = (\Delta_1, \dots, \Delta_n)$ is a predetermined vector such that $x + e_i \Delta_i + e_j \Delta_j \in Q_n$, and

$$f(x + e_i \Delta_i + e_j \Delta_j) = f(x_1, \dots, x_{i-1}, x_i + \Delta_i, x_{i+1}, \dots, x_{j-1}, x_j + \Delta_j, x_{j+1}, \dots, x_n).$$

The quantity EE_{ij} can be used to provide a measure of the effect of the combined-actions between the input parameters X_i and X_j on the model output Y (Mixed elementary effect, MEE), by calculating the following approximation of second partial derivative [10]:

$$\frac{\partial^2 f(x)}{\partial x_i \partial x_j} = dd_{ij}(x) = \frac{f(x + e_i \Delta_i + e_j \Delta_j) - f(x + e_i \Delta_i) - f(x + e_j \Delta_j) + f(x)}{\Delta_i \Delta_j} \quad (2)$$

Then, by adding and subtracting the quantity $f(x)$, we obtain the following approximation:

$$\frac{\partial^2 f(x)}{\partial x_i \partial x_j} \cong EE_{ij} - \frac{1}{\Delta_j} E_i - \frac{1}{\Delta_i} E_j, \quad (3)$$

with the elementary effect $E_i = \partial f / \partial x_i$ (and E_j) being the approximation of partial derivative with respect to input X_i (respectively, X_j). The model must be evaluated at the four following points in the space of input parameters in order to compute dd_{ij} :

$$\text{I: } x = (x_1, \dots, x_n); \quad \text{II: } (x + e_i \Delta_i);$$

$$\text{III: } (x + e_j \Delta_j); \quad \text{IV: } (x + e_i \Delta_i + e_j \Delta_j).$$

For a model containing n input parameters, the number of possible combined-actions of two parameters, given by $\binom{n}{2} = \frac{n(n-1)}{2}$, defined the number of elements of the set $T_{ij} = \{dd_{ij}(x) \mid x \in Q_n\}$. The sensitivity indices of the Morris' extension method (see later equations (4), (5) and (6)) are estimated using the following two sampling strategies (experimental plans). The goal of these experimental designs is to extract randomly a sample of r elements $dd_{ij}^{(1)}, \dots, dd_{ij}^{(r)}$ from each element of the set T_{ij} , $1 \leq i \leq j \leq n$ [9].

Throughout this work, the evaluation of MEE is based on the assumption that the set of MEEs across the trajectories has a continuous and non-skewed distribution, which can be summarized accurately by the measures of mean and median of absolute values of MEE and standard deviation (similar to the elementary effects (EE) of simple Morris method [26]).

2.1.1. Sampling strategy of “Handcuffed Prisoners”

The "Handcuffed Prisoners" design is used when the number of input parameters is even [9], which is a mathematical solution to the graph theory problem, to optimize the number of model evaluations needed to evaluate the second order combined-action effects. By analogy with the sampling scheme for the simple Morris method [8], the basic idea is to construct a multiple trajectory (MT) to estimate the mixed effect dd_{ij} for all $\binom{n}{2}$ pairs of input parameters. MT is constructed by joining together a set of simple trajectories having all the same starting point. MT must retain the properties required by the simple Morris method such that at least one elementary effect E_i per input can be estimated. As in the simple Morris method, each simple trajectory in Q_n corresponds to a simple orientation matrix B_i such that its elements are either 0 or 1. In addition, for each value of $i = 1, 2, \dots, n$, there are two rows of B_i that differ only in the i^{th} entries. For instance, the simple orientation matrix in Q_4 is given by:

$$B_4 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

The matrix MT corresponds to a multiple matrix M_B , which is the junction of several simple orientation matrices. Thus, if each simple orientation matrix B_i has a dimension $m_i -$ by $- n$, MT will correspond to a matrix of multiple orientation M_B (or simply, multiple matrix),

$$M_B = \begin{bmatrix} B_1 \\ B_2 \\ \vdots \\ B_t \end{bmatrix}, \text{ of dimension } (\sum_{i=1}^t m_i) - \text{by} - n.$$

Specifically, the optimal experimental plan (in terms of computational cost) will be that for which the number of simple trajectories used to cover the set $\Gamma = \{(i, j), i < j\}$ is minimum. The construction of a simple matrix B is possible if the pairs contained in the block are handcuffed, i.e. if they form a path $\langle i_1, i_2, \dots, i_n \rangle$. Consider, for example n input parameters and a path such that each pair of two successive points of this path is handcuffed. To estimate the

second-order elementary effect EE_{n-1} for the pair of inputs (X_{n-1}, X_n) , it must use the difference of the values of the function f for the coordinates of $(n+1)^{th}$ and $(n-1)^{th}$ rows of the matrix B . Each path defines a simple orientation matrix B or a simple Morris trajectory, which means that the multiple trajectory is constructed from multiple paths. Each path allows the computation of all second order elementary effects for all pairs of two successive points of this path. In a path, for each input parameter, the combined-actions that are taken into account are with the preceding parameter and the next parameter according to this path. Thus, the objective is to: “Find a partition of I made of $\frac{n}{2} (= s)$ subsets such that each of this subset is composed of $(n-1)$ handcuffed pairs”. These $(n-1)$ handcuffed pairs $\{(i_1, i_2), (i_2, i_3), \dots, (i_{n-1}, i_n)\}$ represents a path designated by $\langle i_1, i_2, \dots, i_n \rangle$, for n being even ($n = 2s$). Finally, in order for a handcuffed design to exist, the following conditions must be satisfied [34]:

- 1) Each element of the set appears among the paths the same number of times;
- 2) Each of n prisoners handcuffed of a path is never handcuffed twice with the same prisoner.
- 3) The design "handcuffed prisoners" exists if and only if n is even ($n = 2s$).

More details have been stated in this case and the case where the number of input parameters of a model n is odd ($n = 2s + 1$) [9].

2.1.2. Sampling strategy of “cycle equitable graphs”

Let us now present the second experimental plan [10]. The computation of a mixed effect of a pair (X_i, X_j) in the directions of (i, j) requires the design of a graph that contains a quadratic cycle:

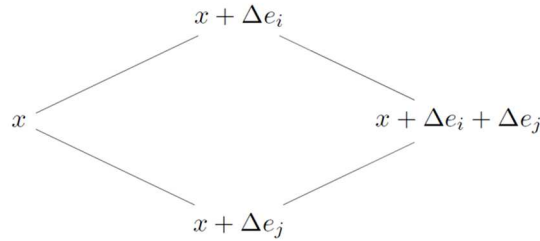


Figure 1: The form of a quadratic cycle [10].

The generic families of graphs that allow the calculation of $c \geq 1$ mixed effect for all possible pairs of two input parameters of a model are called “ (n, c) – cycle equitable graphs”.

Let $S \subset Q_n$ denote the subgraphs of the unit hypercube with dimension $n : Q_n = [0,1]^n$ (where n is the number of input parameters of a model).

- S is said to be a graph of the (n, m) – edge equitable form and represented by $S = G_m^n$ if and only if S has exactly m edges in all the coordinates $i \in \{1, \dots, n\}$ [35].
- $S \subset Q_n$ is said to be a graph of the (n, c) – cycle equitable form and represented by $S = H_c^n$ if and only if S has exactly c quadratic cycles (4–cycles) in each pair of coordinates $(i, j) \in \{1, \dots, n\}^2, i \neq j$.

The subgraphs of Q_n are represented using edge labels (or colors) to indicate the direction along which they are aligned (there will be n different labels in the subgraphs of Q_n).

Figure 2 shows an illustration of this class of graphs of $(5, 1)$ – cycle equitable, i.e. that has exactly one cycle of size 4 involving all 10 possible pairs of input parameters.

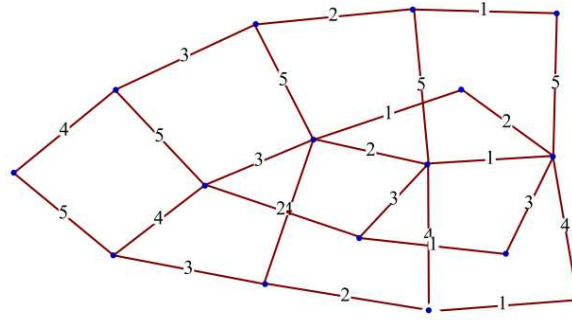


Figure 2 : A subgraph of the form $(5, 1)$ – cycle equitable of Q_5 [10].

Each graph of the form (n, c) – cycle equitable is represented by a matrix. This matrix can be used to construct the sampling matrix and that allows the computation of the mixed effects of the all-possible pairs of input parameters. See [10, 35] for more details.

2.1.3. Sensitivity indices

The experimental plans presented above are used in order to calculate the following classical descriptive measures:

- the mean of MEE :

$$\mu_{ij} = \frac{1}{r} \sum_{l=1}^r dd_{ij}^{(l)} \quad (4)$$

- the standard deviation of MEE :

$$\sigma_\mu = \sqrt{\frac{1}{r} \sum_{l=1}^r (dd_{ij}^{(l)} - \mu_{ij})^2} \quad (5)$$

315 • the mean of absolute values of MEE :

$$\mu_{ij}^* = \frac{1}{r} \sum_{l=1}^r |dd_{ij}^{(l)}| \quad (6)$$

316

317 where r is the number of repetitions of the Morris' extension method, i.e. number of multiple
 318 trajectories. The estimated mean of absolute values μ_{ij}^* of values dd_{ij} is a measure of the relative
 319 importance of the combined-actions of two input parameters, while σ_μ (standard deviation) is
 320 an indicator of the effects of the combined-actions of two input parameters about the presence
 321 or not of non-bilinear effects and / or of combined-actions of order ≥ 3 . Thus, using μ_{ij}^* and σ_μ
 322 we can classify all possible pairs of inputs (X_i, X_j) of the model into three classes according to
 323 their effects and their influence on model output, such that in the Morris method [23]:

324 (C1) If μ_{ij}^* and σ_μ have very low values (close to zero $\simeq 0$), we consider that there's no effect
 325 of combined-action between (X_i, X_j) on the output;

326 (C2) If μ_{ij}^* is high and σ_μ is low, we consider that there is a bilinear effect of combined-action
 327 between (X_i, X_j) on the output;

328 (C3) If σ_μ is high (independently of the value of μ_{ij}^*), we consider that the pair of
 329 inputs (X_i, X_j) has a non-bilinear effect and/or more complex combined-actions (i.e.
 330 combined-action of order > 2 with other inputs) on the output.

331 **Remark.** We now briefly analyze why the behavior of sensitivity indices in the conditions (C1),
 332 (C2) and (C3) enables to distinguish bilinear and non-bilinear effects since these details are not
 333 completely presented in most existing references. For instance, consider the pair of inputs $X =$
 334 (X_i, X_j) with a bilinear combined-action on the model output $Y = f(X) = aX_i + bX_j + cX_iX_j$
 335 with $c > 0$.

336 For a given value $x = (x_i, x_j)$ of the input vector, the MEE of (X_i, X_j) is given by:

$$\begin{aligned} 337 \quad dd_{ij}(x) &= \frac{f(x + e_i\Delta_i + e_j\Delta_j) - f(x + e_i\Delta_i) - f(x + e_j\Delta_j) + f(x)}{\Delta_i\Delta_j} \\ 338 \quad &= \frac{f(x_i + \Delta_i, x_j + \Delta_j) - f(x_i + \Delta_i, x_j) - f(x_i, x_j + \Delta_j) + f(x_i, x_j)}{\Delta_i\Delta_j} \end{aligned}$$

$$= \frac{a(x_i + \Delta_i) + b(x_j + \Delta_j) + c(x_i + \Delta_i)(x_j + \Delta_j) - [a(x_i + \Delta_i) + bx_j + c(x_i + \Delta_i)x_j]}{\Delta_i \Delta_j}$$

$$- \frac{[ax_i + b(x_j + \Delta_j) + cx_i(x_j + \Delta_j)] + ax_i + bx_j + cx_i x_j}{\Delta_i \Delta_j}$$

$$= \frac{c \Delta_i \Delta_j}{\Delta_i \Delta_j} = c = \text{constant}.$$

That results in the following respective values of mean and standard deviation of MEE:

$$\mu_{ij} = \frac{1}{r} \sum_{l=1}^r dd_{ij}^{(l)} = \frac{r \times c}{r} = c = \text{constant} = \mu_{ij}^*.$$

$$\sigma_\mu = \sqrt{\frac{1}{r} \sum_{l=1}^r (dd_{ij}^{(l)} - \mu_{ij})^2} = \frac{1}{r} \sqrt{\sum_{j=1}^r [c - c]^2} = 0.$$

Thus, firstly, for a pair of inputs of class (C1) with values of μ_{ij}^* and σ_μ close to zero (i.e. $c \simeq 0$), we have $Y = f(X) \simeq aX_i + bX_j$, which corresponds to non-bilinear effects of (X_i, X_j) on model output Y . In this case, these two input parameters X_i and X_j have a linear effect on the model output Y . Secondly, for a pair of inputs of class (C2) with a high value of μ_{ij}^* (i.e. $\mu_{ij}^* \gg 0$) and a small value of σ_μ , we have a non-negligible contribution of the term $cX_i X_j$ to model output Y that corresponds to a bilinear effect of (X_i, X_j) . Thirdly, for a pair of inputs of class (C3), the high value of $\sigma_\mu \gg 0$ indicates values of $dd_{ij}(x)$ that are not constant. Thus, the parameter c is not constant and can be assumed as a third variable $c = X_k$, which implies combined-actions of order ≥ 3 of inputs (X_i, X_j, X_k) on model output Y . A similar remark is presented in **Section II** in Supplementary material for the indices of simple Morris method.

In comparison with the classical indices based on mean of MEE, one can also compute the medians γ_{ij} and γ_{ij}^* , respectively, of the mixed effects and absolute values of the mixed effects of the pair of inputs (X_i, X_j) . The indices based on the median of MEE merit to be investigated to classify all possible pairs of inputs (X_i, X_j) , similar to the indices based on the mean of MEE. The objective is take advantage of the median as a more stable statistic measure than the mean, which is particularly less sensitive to the addition of extreme values in a sample. Screening and ranking results will be investigated according to these two types of sensitivity indices.

Finally, by using μ_{ij} we can identify the sense of the influence of each second order combined-action relative to the model response. If $\mu_{ij}(X_i, X_j) < 0$ then the output of the model and the combined-action between (X_i, X_j) vary in the opposite sense. However, the index μ_{ij} is not studied in this paper, as well as the index γ_{ij} . The meaning of the sense of combined-action of a pair of parameters will require to be deeper investigated, regarding to the sense of the individual action of each parameter in the pair.

Note that the ratio σ_μ/μ_{ij}^* is another measure suggested for the classification of the combined-actions influence of the pair of inputs (X_i, X_j) on the output (for more details, see **Section III** in Supplementary Material).

2.2. Sobol method

The calculation of Sobol indices is recognized to be an efficient SA method, but which can have a high computational cost. These indices allow us to quantify the contribution of the variability of individual input parameter or group of input parameters to the variation of the model output [18]. The Sobol method is based on the decomposition of the variance of the model output such that [36]:

$$Y = f_0 + \sum_{i=1}^n f_i(X_i) + \sum_{1 \leq i < j \leq n} f_{i,j}(X_i, X_j) + \dots + f_{i,\dots,n}(X_i, \dots, X_n) \quad (7)$$

Based on the decomposition of the function f of the model in the sum of elementary functions, the variance of Y denoted V can then be decomposed as follows:

$$V = \sum_{i=1}^n V_i + \sum_{1 \leq i < j \leq n} V_{ij} + \dots + V_{1,\dots,n} \quad (8)$$

where

$$V_i = V(E[Y | X_i]),$$

$$V_{ij} = V(E[Y | X_i, X_j]) - V_i - V_j,$$

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

and so on until order n .

The first order Sobol indices S_i measure the effect of the individual inputs such that

$$S_i = \frac{V(E[Y|X_i])}{V(Y)} = \frac{V_i}{V}, \quad (9)$$

while the second-order Sobol indices S_{ij} correspond to the influence of the combined-action between the two input parameters X_i and X_j (by excluding their individual effects) such that

$$S_{ij} = \frac{V_{ij}}{V}, \quad (10)$$

and so on until order n .

The superset importance $S_{i,j}^{super}$ of a pair of inputs (X_i, X_j) is defined as the sum of all Sobol indices with respect to the supersets containing (X_i, X_j) [37-39]. It was calculated by dividing the Total interaction index (TII) $= V_{i,j}^{super}$ on the total variance such that

$$S_{i,j}^{super} = \frac{V_{i,j}^{super}}{V}, \quad (11)$$

with $V_{i,j}^{super} = \sum_{I \supseteq \{i,j\}} V_I = \text{TII}$ where $I \subseteq \{1, \dots, n\}$. For instance, for a model $Y = f(X_1, X_2, X_3, X_4)$, the superset importance $S_{1,2}^{super} = S_{12} + S_{123} + S_{124} + S_{1234}$.

The total interaction index aims to identify the total influence of combined-actions for all possible pairs of influential inputs on the response model, i.e. including the influence of second-order combined-actions and the combined-actions of order > 2 . The calculation of Total interaction indices provides information about the total combined-actions for all possible pairs of model. Sobol indices can be estimated using samplings of input parameters within their interval of variation and according to their probability distribution function. Random samplings such as Monte Carlo method (see [18] for first order and interaction indices and [31] for first order and total indices), or stratified samplings as the quasi Monte Carlo [5], or Latin hypercube, can be used [19]. In this paper, the Sobol sensitivity indices are estimated using the classical Monte-Carlo sampling method. Note that a graphic tool ‘‘FANOVA graph’’ [40] is available in the literature to visualize the structure of the model including their individual and estimated combined-action effects based on Sobol indices.

2.3. Convergence criteria

Three criteria for the assessment of the convergence of the SA results for pairs of input parameters are presented, adapted from SA of individual input parameters [32]. These convergence indicators allow for a rigorous assessment of convergence and comparison of sample sizes across methods, without additional model evaluations. The computation of the convergence criteria required normalized sensitivity indices denoted SI_{ij} , which measure the

combined influence of each input pair (X_i, X_j) on the model output of a model. For the Morris' extension method, we defined normalized measures of the mean μ_{ij}^* and median γ_{ij}^* of absolute values of MEE of Morris' extension method, which can be compared to Sobol indices in $[0,1]$, such that:

$$\beta_{ij}^* = \frac{\mu_{ij}^*}{\max_{1 \leq i < j \leq n} (\mu_{ij}^*)} \in [0,1] \text{ and } \alpha_{ij}^* = \frac{\gamma_{ij}^*}{\max_{1 \leq i < j \leq n} (\gamma_{ij}^*)} \in [0,1] \quad (12)$$

where $\max_{1 \leq i < j \leq n} (\mu_{ij}^*)$ and $\max_{1 \leq i < j \leq n} (\gamma_{ij}^*)$ are the maximum values of μ_{ij}^* and γ_{ij}^* , respectively, for all input pairs possible (X_i, X_j) . These normalized indices still provide semi-quantitative measures of sensitivity. For the second-order and total interaction indices of Sobol, we considered $SI_{ij} = S_{ij}$ and $SI_{ij} = S_{ij}^{Super}$, respectively.

2.3.1. Convergence of the sensitivity indices value

The convergence of the sensitivity indices is reached when the values of the indices remain stable. To assess the convergence of the sensitivity value, we define a quantitative criterion by computing the width of the 95% confidence intervals (5% significance level) of the normalized sensitivity index SI_{ij} . We use the maximum width of the confidence intervals across all the model input pairs as a summary statistic:

$$Stat_{input \text{ pairs indices}} = \max_{1 \leq i < j \leq n} (SI_{ij}^{ub} - SI_{ij}^{lb}), \quad (13)$$

where SI_{ij}^{ub} and SI_{ij}^{lb} are the upper and lower bounds of the normalized sensitivity index SI_{ij} of (X_i, X_j) , with n being the number of model input parameters. The convergence of sensitivity indices value is considered to be reached when the value of $Stat_{input \text{ pairs indices}}$ is lower than 0.05 [32].

2.3.2. Convergence of input pair ranking

The convergence of input pair ranking is achieved if the ordering between the input pairs remains stable. The convergence of input pair ranking can be assessed by using a quantitative criterion. We define for this assessment an adjusted and weighted rank correlation coefficient, which is expressed by:

$$Stat_{input\ pairs\ ranking} = \sum_{1 \leq i < j \leq n} |R_{ij}^{(1)} - R_{ij}^{(2)}| \frac{\max_{(1),(2)}^2(SI_{ij}^{(1)}, SI_{ij}^{(2)})}{\sum_{1 \leq i < j \leq n} (\max_{(1),(2)}^2(SI_{ij}^{(1)}, SI_{ij}^{(2)}))}, \quad (14)$$

where $SI_{ij}^{(1)}$ and $SI_{ij}^{(2)}$ are the values of the normalized sensitivity index SI_{ij} of an input pair (X_i, X_j) estimated using the 1st and 2nd repetitions of the application of the Morris' extension method, respectively and $R_{ij}^{(1)}$ and $R_{ij}^{(2)}$ are their ranks.

This indicator emphasizes the disagreements in the ranking for the most influential input pairs while neglecting the disagreements for the least sensitive input pairs by directly using the sensitivity values to weight rank reversals. We used the squared maximum sensitivity index value between two repetitions of the application of the Morris' extension method.

When the value $Stat_{input\ pairs\ ranking}$ equal to 1 means that, on average, the differences in the ranking for the most influential input pairs are less than one position. So, the convergence of input pair ranking is considered to be reached when the value of $Stat_{input\ pairs\ ranking}$ falls below 1.

2.3.3. Convergence of input pair screening

The convergence of input pair screening is reached if the partitioning between influential and non-influential input pairs stabilizes. In other words, the convergence of input pair screening is reached when the sensitivity indices for the lower-sensitivity input pairs have converged. For the sensitivity indices, we can assume a threshold value T below which the input pairs are considered as non-influential, which results in the subset

$$X_0 = \{(X_i, X_j) \text{ when the sensitivity index } SI_{ij} < T\}, \quad (15)$$

where SI_{ij} is the normalized sensitivity index for the pair (X_i, X_j) . Herein we consider the threshold $T = 5\%$ (as in the case of individual input parameters [32]).

To assess the convergence of input pairs screening, we use as a quantitative criterion the maximum width of the 95% confidence intervals across the lower-sensitivity input pairs in X_0 :

$$Stat_{input\ pairs\ screening} = \max_{(X_i, X_j) \in X_0} (SI_{ij}^{ub} - SI_{ij}^{lb}) \quad (16)$$

Similar to the convergence of sensitivity indices, the convergence of input pairs screening is considered to be reached when the value of $Stat_{input\ pairs\ screening}$ is below 5%.

3. Applications and Results

In the following applications, the Morris' extension method and total interaction Sobol indices are investigated with different numbers of trajectories (r) and simulations (N). We look to determine the optimal number of trajectories and simulations needed to obtain stable results of the sensitivity of the combined-actions between two input parameters of all possible pairs of inputs of the two considered models. The intervals of variation and the probability distributions of input parameters are needed for the application of Morris' extension method and Sobol method, respectively.

3.1. Theoretical model

Consider the simple analytical function with additive bilinear effects such that [9]:

$$f = \sum_{i=1}^4 b_i w_i + \sum_{i \leq j} b_{ij} w_i w_j \quad (17)$$

where $w_i = 2 \times (x_i - \frac{1}{2})$, $x = (x_1, x_2, x_3, x_4) \in [0, 1]^4$. The coefficients b_i and b_{ij} are set to the following standard values: $b_3 = 10$; $b_{22} = 30$; $b_{12} = 80$; $b_{13} = 60$; $b_{14} = 40$. All the other coefficients are taken to be the absolute values of a set of random numbers generated from a normal distribution with zero mean and unit standard deviation. In particular, their values are: $b_1 = 0.05$; $b_2 = 0.59$; $b_4 = 0.21$; $b_{11} = 0.00$; $b_{23} = 0.73$; $b_{24} = 0.18$; $b_{33} = 0.64$; $b_{34} = 0.93$; $b_{44} = 0.06$. The Morris' extension method is applied by incrementally increasing the number of trajectories (r) from 2 to 20 (**Figure 3**), and Sobol method (second-order and total interaction) runs by incrementally increasing the size of classical Monte-Carlo samples (N) from 100 to 5600 (**Figure S11** in Supplementary Material).

For the simple model (17), a small number of trajectories (here, equal to 2) was sufficient to obtain convergent results when applying the Morris' extension method (**Table 2**). When increasing the number of trajectories beyond 2, screening and ranking results of the influence of all possible pairs of input parameters did not vary. Particularly, screening and ranking results of the Morris' extension method were the same using the two possible experimental plans presented in Section 2.1, as well as the indices based on mean and median of MEE (**Figure 3** and **Figure S10** in Supplementary Material).

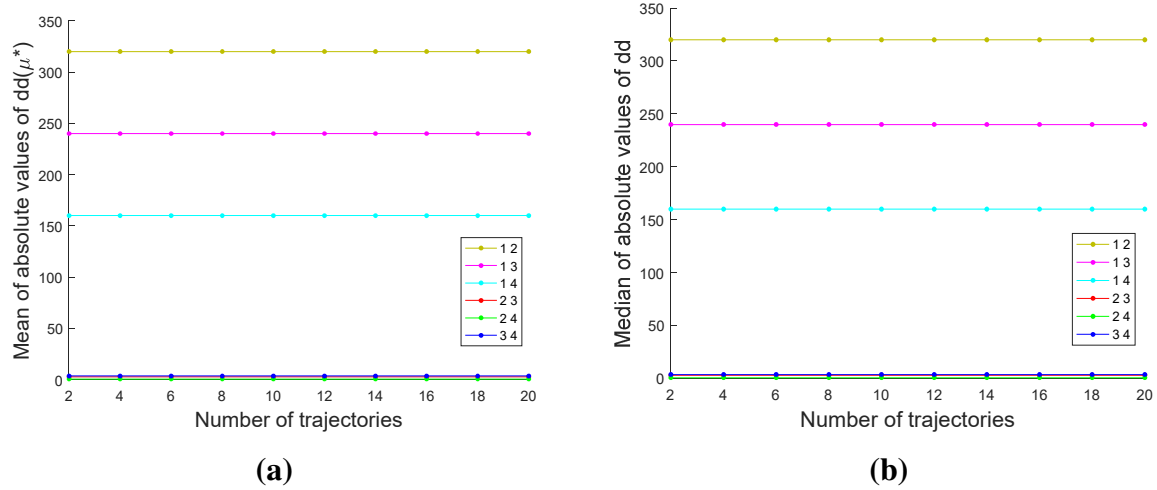


Figure 3 : Variations of the mean (a) and median (b) of absolute values of MEE for pairs of input parameters of the theoretical model by applying the Morris' extension method using the sampling strategy of Handcuffed Prisoners.

Concerning the two indices based on variance decomposition of model output, total interaction indices particularly distinguished more clearly groups of influential and non-influential parameters than second-order Sobol indices (Figure S11 in Supplementary Material). However, the two types of Sobol indices gave the same ranking of influential combined-actions for all possible pairs of input parameters of the theoretical model (17) (Table 2), as the Morris' extension method. A relatively low number of simulations (herein, equal to 100) was sufficient to obtained a ranking that did not vary when increasing the number of simulations for the two types of Sobol sensitivity indices. However, a higher number of simulations was necessary to reach the stability of the two types of sensitivity indices (herein, equal to 4100).

Rank	Methods					
	Morris' extension				Sobol	
	Handcuffed Prisoners Sampling		Cycle equitable Sampling		Second-order Sobol indices	Total interaction indices
	Using Mean	Using Median	Using Mean	Using Median		
1	(X_1, X_2)	(X_1, X_2)	(X_1, X_2)	(X_1, X_2)	(X_1, X_2)	(X_1, X_2)
2	(X_1, X_3)	(X_1, X_3)	(X_1, X_3)	(X_1, X_3)	(X_1, X_3)	(X_1, X_3)
3	(X_1, X_4)	(X_1, X_4)	(X_1, X_4)	(X_1, X_4)	(X_1, X_4)	(X_1, X_4)

Table 2 : Ranking of the first third most influential combined-actions between two inputs obtained by applying the Morris' extension method and interaction Sobol indices on the theoretical model.

Based on the formulas presented in the last column of **Table 1**, we computed the computational cost of Morris' extension and Sobol indices (second-order and total interaction) applied to the theoretical model (**Table 3** and **Table 4**). The number of model evaluations to obtain a stable ranking for the Sobol method (for $N=100$) was around 21 times higher than that for the Morris' extension method (for $r=2$).

	Number of trajectories (r)									
	2	4	6	8	10	12	14	16	18	20
Calculation cost of Morris' extension method	28	56	84	112	140	168	196	224	252	280

Table 3 : The calculation cost according to the number of trajectories used in the application of Morris' extension method to the theoretical model.

	Sample size (N)											
	100	600	1100	1600	2100	2600	3100	3600	4100	4600	5100	5600
Calculation cost of second order and total interaction Sobol indices	600	3600	6600	9600	12600	15600	18600	21600	24600	27600	30600	33600

Table 4 : The calculation cost according to the sample sizes used in the application of second-order and total interaction Sobol indices to the theoretical model.

We do not present formal criteria for the assessment of the convergence of the SA results, which were not relevant for the simple theoretical model.

3.2. Case study: concrete carbonation model

The second illustration concerns a carbonation meta-model that allows calculating the carbonation depth in concrete structures (**Figure 4**) [33]. The carbonation in concrete is a major cause of the corrosion of reinforced concrete structures. It is one of several pathologies that can affect concrete; the remedy against this pathology plays an important role in improving the durability of concrete. The developed carbonation model is governed by the diffusion of carbon dioxide (CO_2) in concrete that is based on the analytic solution of the Fick's first law in the form [41]:

$$x_{CO_2} = A \cdot \sqrt{t} \quad (18)$$

The carbonation front depth $x_{CO_2}(m)$ depends on the exposure time t (s) and the carbonation coefficient A ($m/s^{1/2}$) that is determined by:

$$A = f(RH, T, CO_2, C, W/C, S/G, S_{max}, CEM, f_{cem}, t_c) = \sqrt{\frac{2 \cdot D_{CO_2} \cdot [CO_2]_{ext}}{a}} \quad (19)$$

where D_{CO_2} (m^2/s) is the CO_2 -diffusion coefficient in carbonated concrete, a (kg/m^3) is the amount of CO_2 absorbed in a unit volume of concrete. When the carbonation depth x_{CO_2} is equal to the concrete cover depth (d), the service life (t_{ser}) that corresponds to the corrosion initiation time is expressed as:

$$t_{ser} = \frac{d^2}{A^2} \quad (20)$$

Ta et al. [33] used this model to identify the individual effects of the input parameters on the corrosion initiation time, by using simple Morris method and Sobol SA method. However, non-negligible effects of combined-actions of inputs of carbonation model were pointed out on the corrosion initiation time but still remain to be studied. Summary descriptive statistics (mean, min: minimum, max: maximum, COV: the variation coefficient) and the probability distribution of the input parameters are given in the **Table 5**.

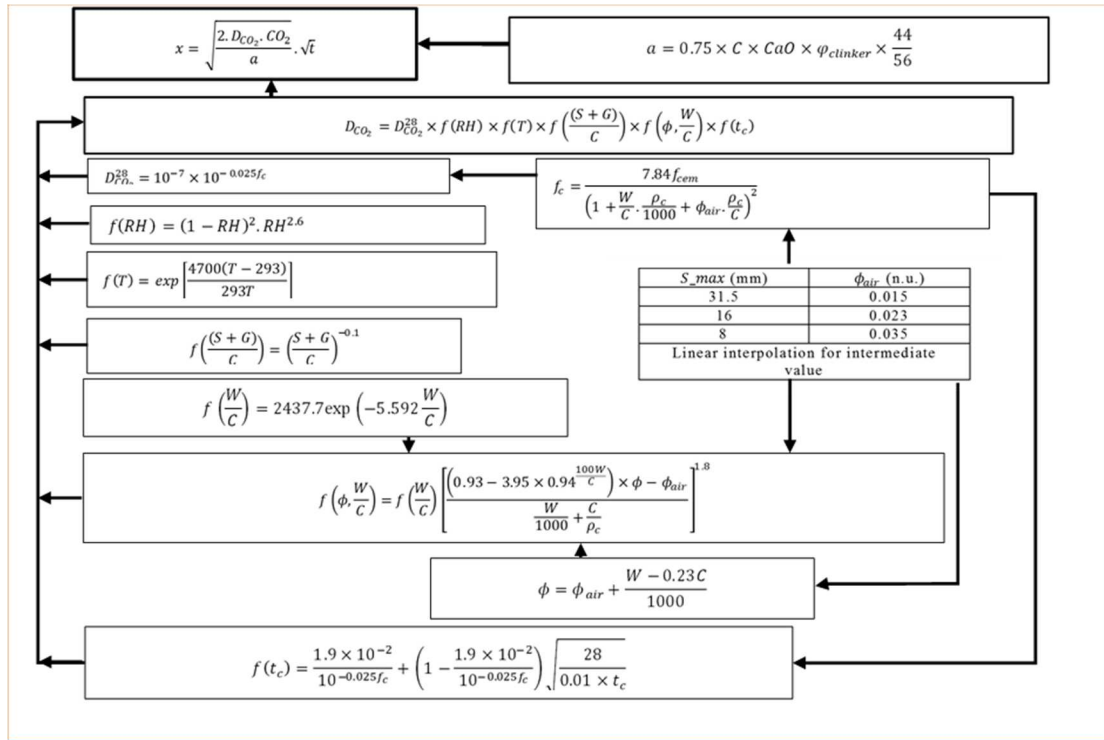


Figure 4 : Meta-model for calculating the depth of carbonation front [33].

Input Parameters	Unit	Mean	Min	Max	COV	Distribution
d	M	0,065	0,05	0,08		Uniform
t_c	Days	2	1	3		Uniform
S_max	Mm	26	20	32		Uniform
C	kg/m ³	404,5	300	509		Uniform
W/C	No unit	0,45	0,4	0,5		Uniform
S/G	No unit	1,3	0,5	2,1		Uniform
f_{cem}	MPa					Discrete Uniform(3 strength classes)
CEM	No unit					Discrete Uniform(10 cement types)
T	K	287,4	272,4	309,1	0,03	Truncated Normal
RH	No unit	0,56	0,2	0,88	0,33	Truncated Normal
CO ₂	Ppm	380	304,5 6	456,8	0,05	Truncated Normal

Table 5 : Statistical description of the input parameters of the carbonation model [33].

The Morris' extension method was applied by incrementally increasing the number of trajectories from 100 to 4600. The mean absolute deviation $E_{\mu^*} = \frac{1}{r} \sum_{l=1}^r |dd_{ij}^{(l)}| - \mu_{ij}^*$ and median absolute deviation $E_{\gamma^*} = \frac{1}{r} \sum_{l=1}^r |dd_{ij}^{(l)}| - \gamma_{ij}^*$ were calculated to evaluate how sensitivity indices μ_{ij}^* and γ_{ij}^* are representative or not of dd_{ij} values. We presented the difference $E_{\mu^*} - E_{\gamma^*}$ for the most influential pairs of inputs (**Figure 6**); see also **Table S10** in Supplementary material. The Sobol method for second-order was run by incrementally increasing the size of classical Monte-Carlo samples from 10000 to 510000, while the Sobol method for total interaction was run by incrementally increasing the size of classical Monte-Carlo samples from 100 to 9100.

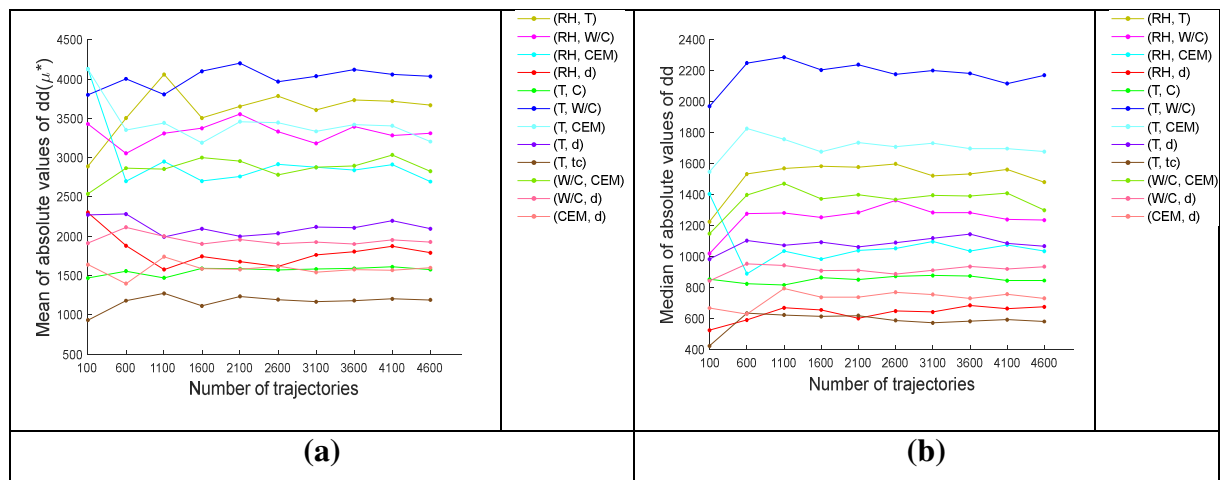
3.2.1. Results of Morris' extension method

The number of trajectories required to obtain convergent results was obviously higher than previously for the simple theoretical model, when applying the Morris' extension method

based on the sampling strategy of Handcuffed Prisoners on the carbonation model. The magnitude of indices based on the mean of MEE enables to quickly distinguish influential and non-influential groups of input pairs of carbonation model, from the minimum number of trajectories considered (herein, equal to 100, **Figure 5(a)**). Comparatively, the magnitude of indices based on the median of MEE rather points out clearly the most influential pairs of inputs (**Figure 5(b)**).

The criteria in Section 2.3 were implemented to assess the three types of convergence. The convergence of screening results of input pairs was achieved from 110 and 150 trajectories when using indices γ_{ij}^* and μ_{ij}^* based on median and mean of MEE, respectively (**Figure S12** in Supplementary Material). Then, the convergence of ranking results was achieved from around 2,600 trajectories with indices γ_{ij}^* based on the median of MEE, whereas more than 4,600 were required to achieve this convergence with indices μ_{ij}^* based on the mean of MEE (**Figure S13** and **Figure S14** in Supplementary Material). The influential pairs of inputs were globally the same using the indices based on the mean and median of MEE but with little changes in their relative ranking (**Table 6**). The convergence of values of indices γ_{ij}^* and μ_{ij}^* was achieved from a similar number of 14100 trajectories (**Figure S15** in Supplementary Material).

Note that results obtained from the Morris' extension method were completely different when applying the two sampling strategies (Handcuffed prisoners and cycle equitable graphs) on the corrosion initiation time model (**Table 6**). Results obtained by using the sampling strategy of cycle equitable graphs are illustrated in Supplementary Material (**Figure S16** and **Figure S17**).



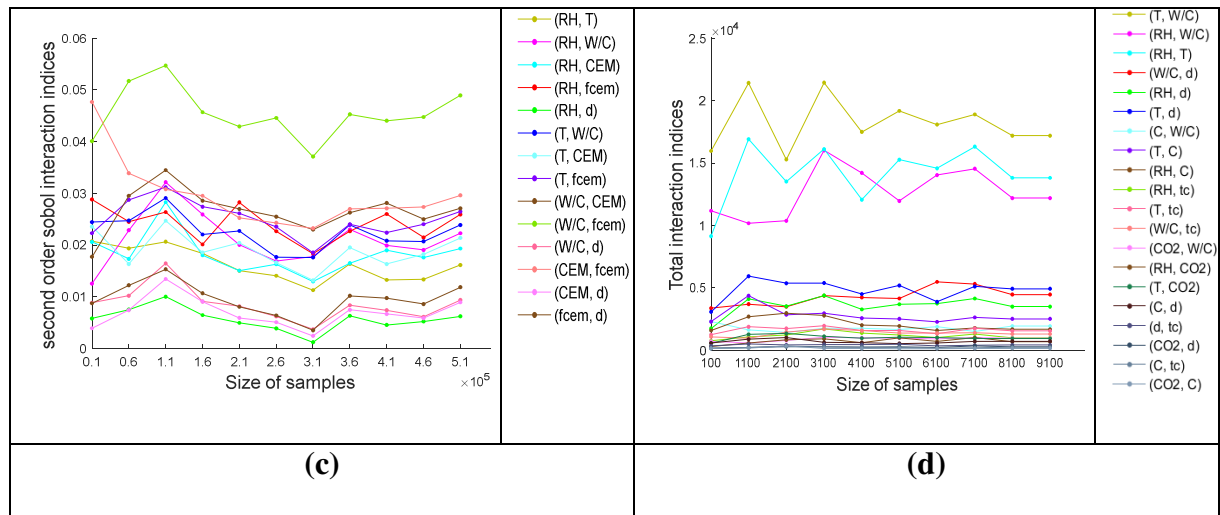


Figure 5: Indices μ_{ij}^* (a) and γ_{ij}^* (b) of the Morris' extension method using the sampling strategy of Handcuffed Prisoners and second-order (c) and total interaction indices (d) of Sobol, for input pairs of carbonation model [33].

Rank	Methods					
	Morris' extension				Sobol	
	Handcuffed Prisoners Sampling		Cycle equitable Sampling		Second-order Sobol indices	Total interaction indices
	Using Mean	Using Median	Using Mean	Using Median		
1	(T, W/C)	(T, W/C)	(d, t_c)	(d, t_c)	(W/C, f_{cem})	(T, W/C)
2	(RH, T)	(T, CEM)	(T, d)	(T, d)	(CEM, f_{cem})	(RH, T)
3	(RH, W/C)	(RH, T)	(W/C, t_c)	(W/C, t_c)	(W/C, CEM)	(RH, W/C)
4	(T, CEM)	(W/C, CEM)	(T, W/C)	(T, CEM)	(T, W/C)	(T, d)
5	(W/C, CEM)	(RH, W/C)	(T, CEM)	(T, W/C)	(RH, CEM)	(W/C, d)
6	(RH, CEM)	(RH, CEM)	(RH, W/C)	(RH, W/C)	(RH, W/C)	(RH, d)

Table 6 : Ranking of the most influential combined-actions between two inputs obtained by applying the Morris' extension method and Sobol indices on the carbonation model.

Moreover, the cost associated with the calculation of the indices of the Morris' extension method was given in **Table 7**. The calculation cost required to obtain stable ranking with indices γ_{ij}^* based on the median of MEE (for $r=2,600$) was around 2 times higher than that with indices μ_{ij}^* based on the mean of MEE (for $r=4,600$). The computational cost for the calculation of the indices of the Morris method (the influences for the single inputs) was given in Supplementary Material (**Table S11**), for comparison purposes. Likewise, additional graphs showing the variations of Morris indices and the evolution of ranking of individual inputs of the carbonation model according to their relative importance are given in Supplementary Material (**Figure S19** and in **Figure S20**).

Number of trajectories (r)

	100	600	1100	1600	2100	2600	3100	3600	4100	4600
Calculation cost of Morris' extension method	9200	55200	101200	147200	193200	239200	285200	331200	377200	423200

Table 7 : The calculation cost according to the number of trajectories used in the application of Morris' extension method to the carbonation model.

Finally, concerning the Morris' extension method, the difference $E_{\mu^*} - E_{\gamma^*}$ was found to be always positive for all pairs (X_i, X_j) , reflecting that the median value γ_{ij}^* was better able to represent the absolute values of MEE than the mean value μ_{ij}^* (**Figure 6**); see also **Table S10** in Supplementary material.

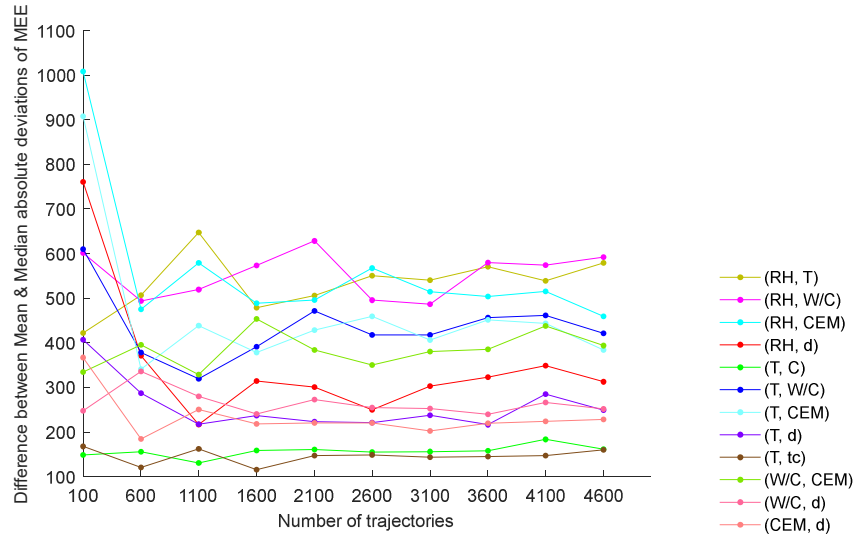


Figure 6: The difference $E_{\mu^*} - E_{\gamma^*}$ of mixed elementary effects (MEE) of the most influential pairs of inputs on the carbonation model.

3.2.2. Results of second-order and total interaction Sobol indices

Concerning the two indices based on variance decomposition of model output, the magnitude of total interaction indices enabled to distinguish influential and non-influential groups of pairs of inputs from the minimum number of samples considered (herein, equal to 100, **Figure 5(d)**). Comparatively, the magnitude of second-order Sobol indices pointed out the most influential pair of inputs (**Figure 5(c)**). The ranking of the first third most influential pairs of inputs was achieved through convergent sensitivity indices with a smaller sample size (herein, 5,100) for total interaction sensitivity indices than for second-order indices (herein, 460,000) (**Figure S18** in Supplementary material). Likewise, to achieve the convergence of total interaction sensitivity indices would require a smaller sample size than second order

sensitivity indices. For instance, values of total interaction sensitivity indices of first third most influential pairs of inputs achieved stability around the sample size 8,100. Visual checks of the convergence of SA results were confirmed by implementing formal criteria to assess the three types of convergence (Section 2.3).

The computational cost according to the sample sizes used in the applications of Sobol indices (second-order and total interaction) to the carbonation model are respectively given in **Table 8** and **Table 9**. The number of model evaluations required to obtain a stable ranking for second-order indices (for $N=460,000$) was around 90 times higher than that for total interaction sensitivity indices (for $N=5,100$). Likewise, the minimal number of model evaluations required to obtain a stable ranking for the Morris' extension method with indices γ_{ij}^* based on the median of MEE (for $r=2,600$, **Table 7**) was around 4 times higher than that for total interaction sensitivity indices.

	Sample size (N)										
	10000	60000	110000	160000	210000	260000	310000	360000	410000	460000	510000
Calculation cost of second order Sobol indices	120000	720000	1320000	1920000	2520000	3120000	3720000	4320000	4920000	5520000	6120000

Table 8 : The calculation cost according to the sample sizes used in the application of second-order Sobol indices to the carbonation model.

	Sample size (N)									
	100	1100	2100	3100	4100	5100	6100	7100	8100	9100
Calculation cost of total interaction indices of Sobol	1200	13200	25200	37200	49200	61200	73200	85200	97200	109200

Table 9 : The calculation cost according to the sample sizes used in the application of total interaction indices of Sobol to the carbonation model.

Note that the structure of the carbonation model was visualized using FANOVA graph based on Sobol indices (**Figure S9** in Supplementary material).

4. Discussions and interpretations

4.1. Convergence of combined influences results

Convergence of input pairs screening. Applying the Morris' extension method based on the sampling strategy of Handcuffed Prisoners showed the choice between either (a) indices

based on the mean of MEE to distinguish groups of influential and non-influential pairs of input parameters or (b) indices based on the median of MEE to point out the most influential pairs of input parameters. For the simple theoretical model with additive bilinear effects and the complex civil engineering model with non-bilinear effects, the two types of sensitivity indices revealed the same most influential pairs of parameters. However, a lower number of trajectories was obviously required to provide convergent results for the simple model than for the complex model. For instance, a number of trajectories equal to 10 was chosen in the Morris' extension method for screening relative importance of pairs of 12 input parameters of an energy building model using sensitivity indices based on the mean of MEE [23]. Sobol indices may be also used to distinguish the group of influential and non-influential parameters with respect to their total interaction effect, but with a higher computational cost than the Morris' extension method.

Convergence of input pairs ranking. For the Morris' extension method based on the sampling strategy of Handcuffed Prisoners, using indices based on the median of MEE was more appropriate to obtain a convergent ordering of pairs of inputs with respect to their relative importance. Comparatively, using indices based on the mean of MEE required a higher number of trajectories to achieve stability of the ordering, when applying Morris' extension method with the sampling strategy of Handcuffed Prisoners. Total interaction Sobol indices and indices based on the mean of MEE provide the same ranking of relative importance of the first third influential pairs of inputs, which is different from the ranking provided by second-order Sobol indices. Thus, Morris' extension method revealed the relative importance of most influential pairs of inputs according to their total interaction effect on model output (including second and higher order combined-effects). However, a stable ranking of inputs of carbonation model was achieved with a smaller computational cost for the total interaction Sobol indices than the Morris' extension method. The Morris' extension method, second-order and total interaction Sobol indices had similar results for the theoretical model since this model had not third or higher combined-effects of inputs, unlike the carbonation model.

Convergence of sensitivity indices value. For all the sensitivity analysis methods applied in this work, to achieve stability of sensitivity indices required more model evaluations than to achieve stable screening and ranking results, according to the degree of complexity of the model. For instance, according to total interactions indices, while a sample size of 100 was found to be suitable for screening for the carbonation model, a sample size of 5,100 enabled to rank order first third more influential pairs of parameters but a sample size of 8,100 was required to obtain convergent sensitivity indices. Thus, most of the studies used the Morris methods with low numbers of trajectories that allow achieving a correct distinction of the relative importance

of inputs, i.e. high-, mid- and low-ranked parameters, although the results are not completely stable [42].

Number of trajectories for Morris' methods and sample size for Sobol indices. Choices of number of trajectories r for Morris and Morris' extension method and sample size N for Sobol indices and indices based on the derivatives can be found in the literature. For instance, the number r was typically set between 10 and 50 for studying the influence of input parameters using the simple Morris method [22]. Likewise, a low number of trajectories ($r = 10$) was sufficient to screen out the influential and non-influential pairs according to their relative interactions using Morris' extension method [23]. However, our results showed that whether a low number of trajectories can be suitable for screening, it can be insufficient for input ranking, particularly for complex models (see also [26]). When using the Sobol method, different values of the base sample size are found for the same method when applied to different models within a given type of convergence. For instance, to ensure the convergence of Sobol' indices, one base sample size N of 8,192 was used for a case study with 18 input parameters [43], while another sample size N of 3,000 was used for a case study with 5 input parameters [44]. Likewise, a base sample size of 12,000 was found to be necessary to ensure the convergence of Sobol' indices in a specific case study on complex environmental model, but a much smaller sample size ($N < 2,000$) was sufficient if one was only interested in ranking the most influential input parameters [45]. Moreover, for estimating Sobol' indices on a flood model, a sample size N of 10,000 was used for a case study with 5 input parameters [20]. Note that DGSM were efficiently estimated in most of the cases using quasi-Monte Carlo samples (of size 100 to 1,000) [21].

In our study, for the application of Morris' extension method on the carbonation model, a number of trajectories $r = 110$ was sufficient to reach the convergence of input pairs screening, while $r = 2600$ and $r = 14100$ were sufficient to obtain convergent results of input pairs ranking and sensitivity indices values, respectively. However, for the application of Sobol method on the carbonation model, when using the total interaction indices a sample size $N = 100$ was sufficient to reach the convergence of input pairs screening but the ranking of the third most influential pairs was achieved from $N = 5600$, while $N = 8100$ was sufficient to obtain convergent results of values of sensitivity indices. Moreover, a sample size $N = 460,000$ was sufficient to achieve the convergence of input pairs ranking when using the second-order Sobol indices.

4.2. Recommendations

Guidance on the application of second-order or total interaction indices. In the case of a simple model, the application of Morris' extension method using indices based on the mean or median gave the same results with the same calculation cost in order to screen and rank the most influential pairs of parameters on the response of the model. In addition, the two sampling strategies "Handcuffed Prisoners" and "cycle equitable graphs" can be used.

When the model is complex with no-bilinear effects, the Morris' extension method using indices based on median may be just used to screen out the most influential pairs of parameters, because its calculation cost (i.e. which is a function with respect of number of trajectories and of number of input variables) is lower than indices based on mean. The two types of indices revealed the same group of most influential input pairs. However, as in our civil engineering model, the Morris' extension method using indices based on mean and the total interaction Sobol indices that allow quantifying the total contribution of variability of a pair of inputs to the total variance of the model response gave the same ranking of the most influential pairs of inputs. Thus, the Morris' extension method provides information about the total combined-action influence for most influential pairs of model inputs.

The sensitivity indices of Morris' extension method and the total interaction Sobol indices gave the same results of the total combined influence of input pairs on the model response. However, to apply Sobol method is more costly than the Morris' extension method. Thus, the choice between applying these two methods depends on the main researched information between screening, ranking and quantification of sensitivity indices of input pairs.

Remarks: (1) For the carbonation model, the extension of Morris method based on the sampling strategy of "cycle equitable graphs" [10] provided results completely different from those of the other methods. The sampling strategy of cycle equitable graphs seemed not adequate for a complex model. Deeper investigations are required on the failure of this sampling strategy.

(2) The calculation cost of the application of second-order Sobol indices on complex model is expensive compared with other methods such as the extension of Morris method and the computation of total interaction indices. Therefore, in order to identify the pairs that have the more relative importance on the model response, we can apply the Morris' extension method and compute the total interaction indices, which let us detect the total influence of all possible pairs of the model with not expensive calculation cost. Computational effort is a fundamental

issue associated with any sensitivity analysis technique. Surrogate models is one obvious technique that has been used in past to reduce computational burden associated with sensitivity analysis. For instance, for evaluating the Sobol indices at low computational cost, [46] introduced a novel approach, by post-processing the coefficients of polynomial meta-models belonging to the class of low-rank tensor approximations. Moreover, for CPU-demanding models such as finite element models, [47] proposed an optimized regression approach to compute the polynomial chaos (PC) expansion coefficients using a limited number of evaluations of the true model. However, for evaluating the moment independent sensitivity indices (PDF and CDF based) at low computational cost, [48] proposed a novel approach that integrates hybrid polynomial correlated function expansion (H-PCFE) into the framework of moment independent sensitivity analysis. H-PCFE is a novel surrogate model formulated by coupling polynomial correlated function expansion (PCFE) with kriging. In a similar way to the previous approach, [49] presented a method that couples PCFE with distribution based sensitivity analysis (DSA). By integrating PCFE into DSA, it is possible to considerably alleviate the computational burden.

Combination of 1st, 2nd, and higher order sensitivity analysis. The 1st, 2nd, and higher order analyses should be applied successively using the appropriate sensitivity analysis methods (**Figure 7**), in order to obtain all information concerning the individual and combined-actions effects of input parameters or group of inputs on the model response. More precisely, the 1st order sensitivity analysis method as simple Morris should be applied in order to identify the non-important input parameters. Then, these non-influential inputs should be fixed and the 2nd and higher order sensitivity analysis methods as the Morris' extension method and the Sobol method (second-order Sobol and Total interaction indices) should be performed in order to identify the influential combined-actions of pairs of inputs on the response model.

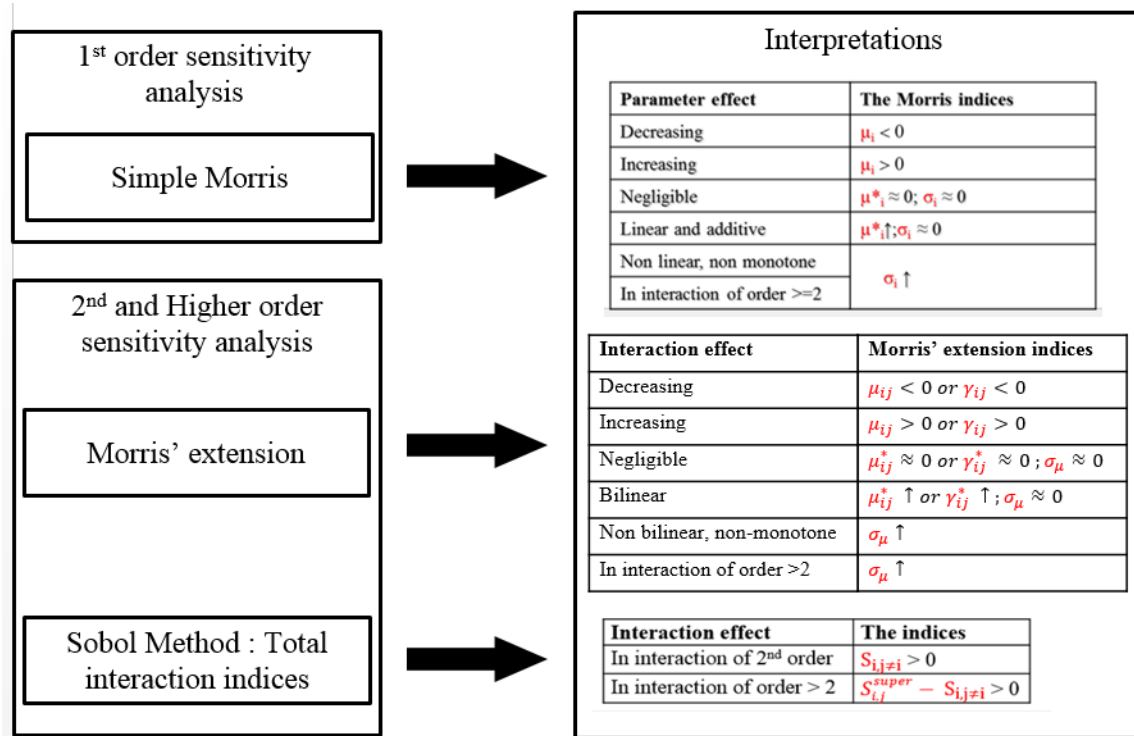


Figure 7 : An illustration of the combination of the 1st, 2nd, and higher order sensitivity analysis. (Notation: $\uparrow$ means that the value is high).

5. Conclusions

This paper investigates the cost-effectiveness and efficiency of the Morris' extension method and the Sobol method to perform second-order and total interaction sensitivity analysis studies. The following issues are raised concerning sensitivity analysis methods: how to choose an adequate number of trajectories and sample size to distinguish influential and non-influential pairs of inputs, how to order pairs of inputs according to their relative importance and how to obtain stable values of sensitivity indices? Applied to the analysis of complex models with the Morris' extension method, simulation results showed that indices based on the median of MEE were competing with classical indices based on the mean of MEE, to screen out the more influential combined-actions on the model response with lower calculation cost. In addition, the Morris' extension method provides information about the total combined-action influence of most influential pairs of model inputs, as the total interaction Sobol indices. As an applied case study, the application of Morris' extension method for a carbonation propagation model showed the joint influence of environmental and technological parameters on the service life of concrete structures, through the influence of coupling between temperature and water / cement ratio.

This work contributes to providing guidance to support practitioners for conducting a sensitivity analysis of a second-order and total interaction of all possible model input pairs. All these issues depend on the degree of complexity of the model studied, i.e. whether there are bilinear or non-bilinear effects and combined-actions of two or more input parameters. Some research prospects should include the study of the sense (or trend) of the combined-action influence for all possible pairs of inputs on the response of model, from the Morris' extension method. That would be an additional valuable information on the sense of the influence of pairs of inputs on the model response when the two inputs vary in the same sense (increasing or decreasing) and in opposite senses.

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Supplementary Material

Sensitivity analysis methods for combined-actions of input parameters in a model

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In this paper, we provide our supplementary material, which includes more information and interpretations of our work by showing additional graphs and tables for our results. This additional material is used to support our main work.

I. Review of Morris method

The Morris method consists of repeating r times an experimental OAT plan. It varies a single parameter at a time randomly by repeating this step r times. It can be seen as a statistical analysis of the empirical estimates of the approximations of partial derivatives (or variations) of an output of the model with respect to each input parameter. This method is used to produce

a qualitative classification of the input parameters. It is a very effective approach that identifies the important input parameters of a model and those that are not influential.

This method performs a number r of local measurements in different points $x^{(1)}, \dots, x^{(r)}$ chosen randomly to cover the whole space of the input parameters Q_n , to measure the main effect of each input parameter by calculating their average, which reduces the dependence of the measure at a given nominal point.

This method is based on the discretization of each input variable to obtain p levels (values) between 0 and 1, i.e. it may take as a value $\{0, 1/(p-1), 2/(p-1), \dots, 1\}$. Each input parameter is assumed to have a uniform distribution $[0, 1]$ and therefore the space of input parameters Q_n is a unit hypercube of dimension n (n being the number of input parameters). If an input parameter X_i has a uniform distribution in $[x_{min}(i), x_{max}(i)]$, it should to transform this input in $[0, 1]$ by using this formula: $\frac{x_i - x_{min}(i)}{x_{max}(i) - x_{min}(i)}$ (where $x_{min}(i)$, $x_{max}(i)$, and x_i are the minimum, the maximum and the value of the input parameter X_i , respectively). We define in the hypercube Q_n a trajectory as a set of $(n+1)$ successive points. Each point differs from the preceding one only by a single coordinate, such that each component is changed only once by a value $\Delta = p/2(p-1)$, then the elementary effect of the input parameter X_i is defined by:

$$E_i(x) = \frac{f(x_1, \dots, x_{i-1}, x_i \pm \Delta, x_{i+1}, \dots, x_n) - f(x)}{\Delta} \quad (1)$$

Where $x \in Q_n$ and $x \pm \Delta \in Q_n$. We can obtain a finite distribution F_i of the elementary effects of X_i by sampling x in Q_n r times.

The mean

$$\mu_i = \frac{1}{r} \sum_{j=1}^r E_i(x^j) \quad (2)$$

And the standard deviation

$$\sigma_i = \sqrt{\frac{1}{r} \sum_{j=1}^r [E_i(x^j) - \mu_i]^2} \quad (3)$$

of the distribution F_i give indications on the influence of input parameter X_i on the output of the model.

The computational cost (the number of required simulation runs) of this method depend on the number of input parameters n and number of trajectories r and it is given by $r * (n + 1)$.

The input parameters of a model identified as non-influential can be set at their nominal value (Mean) and allowing reducing the model and thus obtaining a model with fewer input parameters to calibrate.

II. Distinction of linear and non-linear effects for Morris method

We now briefly describe why the sensitivity indices of simple Morris method enable to distinguish linear and non-linear effects on the model output. For instance, consider the input X_i with a linear individual effect on the model output $Y = f(X) = aX_i + b$.

For a given value $x = x_i$ of the input vector, the simple elementary effect of X_i is given by:

$$E_i(x) = E_i(x_i) = \frac{f(x_i + \Delta) - f(x_i)}{\Delta} = \frac{a(x_i + \Delta) + b - ax_i - b}{\Delta} = \frac{a(\Delta)}{\Delta} = a = \text{constant}.$$

That results in the following respective values of mean and standard deviation of simple elementary effects:

$$\mu_i = \frac{1}{r} \sum_{j=1}^r E_i(x_i^j) = \frac{r \times a}{r} = a = \text{constant} = \mu_i^*$$

$$\sigma_i = \sqrt{\frac{1}{r} \sum_{j=1}^r [E_i(x_i^j) - \mu_i]^2} = \frac{1}{r} \sqrt{\sum_{j=1}^r [a - a]^2} = 0.$$

Thus, firstly, for an input of class (1) with values of μ_i^* and σ_i close to zero (i.e. $a \simeq 0$), we have $Y = f(X) \simeq b$, which corresponds to the negligible effect of X_i on model output Y . Secondly, for an input of class (2) with the high value of μ_i^* (i.e. $\mu_i^* \gg 0$) and low value of σ_i , we have a non-negligible contribution of the term aX_i to model output Y that corresponds to a linear effect of X_i . Thirdly, for an input of class (3), the high value of $\sigma_i \gg 0$ indicates values of $E_i(x)$ that are not constant. Thus, the parameter a is not constant and can be assumed to be

a second variable $a = X_j$, which implies combined-actions of order ≥ 2 of inputs (X_i, X_j) on model output Y .

III. Another measure of Morris' extension method

The mean μ_{ij}^* of absolute values of MEE was introduced above as a measure of importance (combined influence) for the input pair (X_i, X_j) . This information can be complemented by the ratio σ_μ/μ_{ij}^* as an indicator of the shape of combined influence for all possible pairs, i.e. bilinear or non-bilinear effects, as justified below:

- If $\sigma_\mu/\mu_{ij}^* < 0.1$, we consider that the pair of inputs (X_i, X_j) is influential and that it has a bilinear or quasi-bilinear effect.
- If $0.1 < \sigma_\mu/\mu_{ij}^* < 0.5$, we consider that the pair of inputs (X_i, X_j) has a monotonic effect.
- If $0.5 < \sigma_\mu/\mu_{ij}^* < 1$, we consider that the pair of inputs (X_i, X_j) has an almost monotonic effect.
- If $\sigma_\mu/\mu_{ij}^* > 1$, we consider that the pair of inputs (X_i, X_j) has non-bilinear effect and / or combined-actions of order > 2 with the other input parameters.

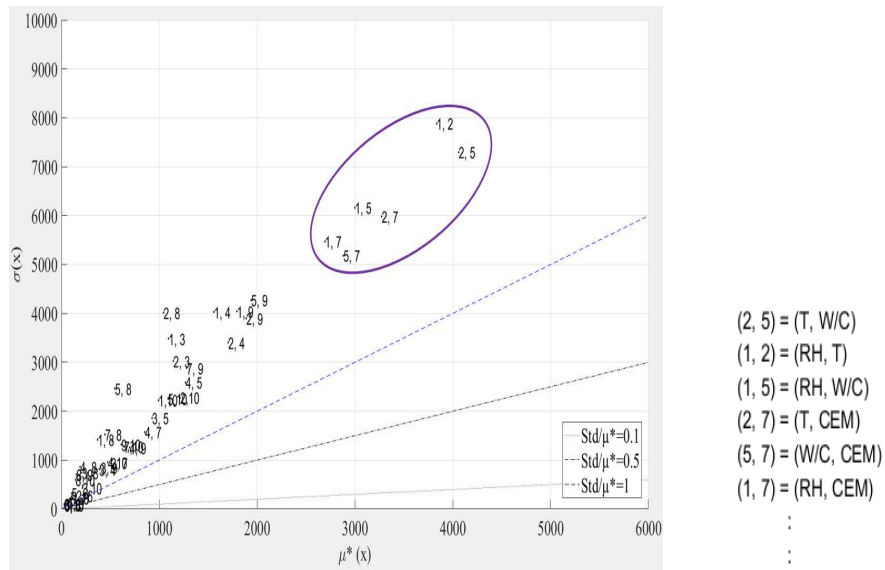


Figure S8 : The calculation of the ratio σ_μ/μ_{ij}^* of Morris' extension method for all possible input pairs of the carbonation model.

Note that the ratio σ_μ/μ_{ij}^* was more than 1 for all possible influential pairs of inputs of the carbonation model such that these pairs had a non-bilinear effect and / or combined-actions of order > 2 with the other input parameters (**Figure S8**). In this figure, we applied the Morris' extension method with number of trajectories $r = 150$, because from this number we could

screening out the input pairs that have most influential combined-actions on the carbonation model.

IV. FANOVA graph

The FANOVA graph is a nice way to visualize the estimated interaction structure. In this graph, each vertex represents one input parameter and an edge between two vertices indicates the presence of second or higher-order interactions between the input parameters. The thickness of the edges is proportional to the total interaction index (TII) and in addition, the thickness of the circles around vertices indicates the first-order indices. The early inactive inputs can be detected as single thin vertices. The FANOVA graph is intended as a tool supporting structural kernel design in the context of non-parametric modelling using Gaussian processes (kriging), whose complexity and performance can improve if the kernel's structure closely reflects the clique structure of the FANOVA graph. Being based on Sobol indices, the set of total variation indices that the FANOVA graph describes are computed by Monte Carlo techniques, and thus they inherit the complexity of Sobol indices.

The two FANOVA graphs of our models are shown below (**Figure S9**).

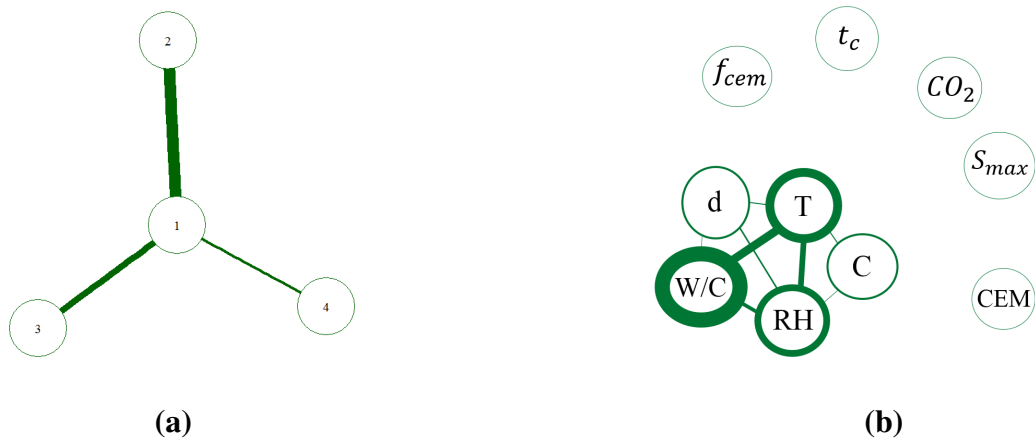
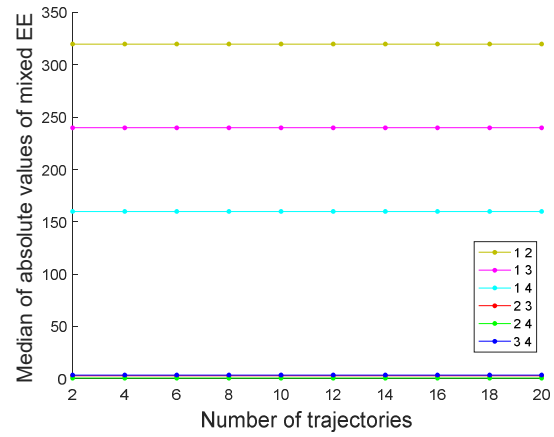
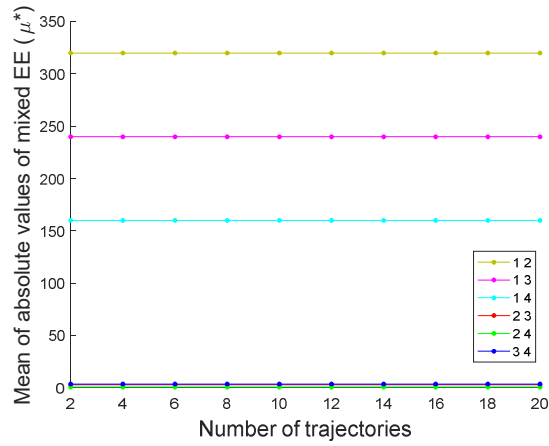


Figure S9 : (a) and (b) are the FANOVA graphs of the theoretical and carbonation models, respectively.

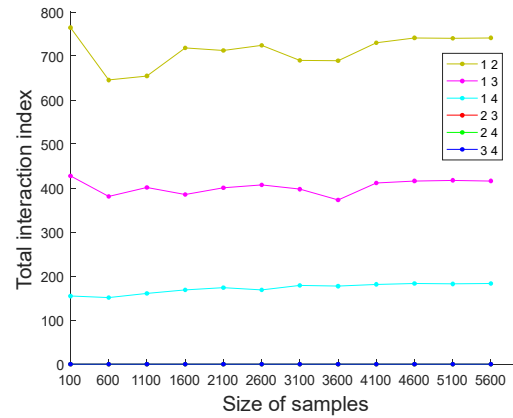
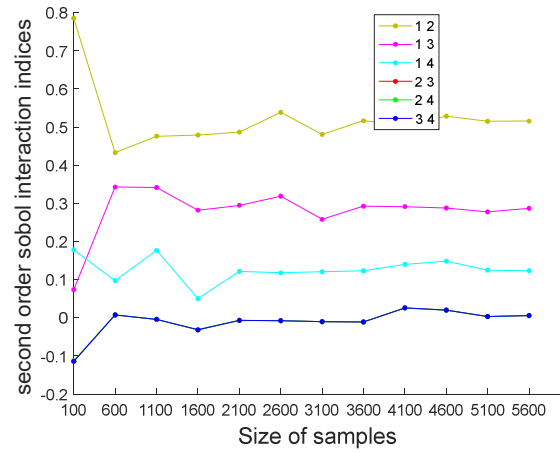
V. Additional graphs and tables



(a)

(b)

Figure S10 : Variations of the mean (a) and median (b) of absolute values of MEE for pairs of input parameters of the theoretical model by applying the Morris' extension method using the sampling strategy of cycle equitable graphs [10].



(a)

(b)

Figure S11 : Variations of the second-order (a) and total (b) interaction Sobol indices of pairs of input parameters of the theoretical model.

r	100	600	1100	1600	2100	2600	3100	3600	4100	4600
Pairs										
(T, W/C)	609	378	320	391	471	417	417	456	461	421
(RH, T)	422	506	647	478	506	550	540	570	539	579
(RH, W/C)	601	494	519	573	628	495	487	579	574	592
(T, CEM)	907	341	438	378	428	459	406	451	444	384
(W/C, CEM)	334	395	328	454	384	350	380	385	437	394
(RH, CEM)	1008	475	579	489	496	567	515	504	515	459

Table S10: The values of the difference ($E_{\mu^*} - E_{\gamma^*}$) of mixed elementary effects (MEE) of the most influential pairs of inputs on the carbonation model.

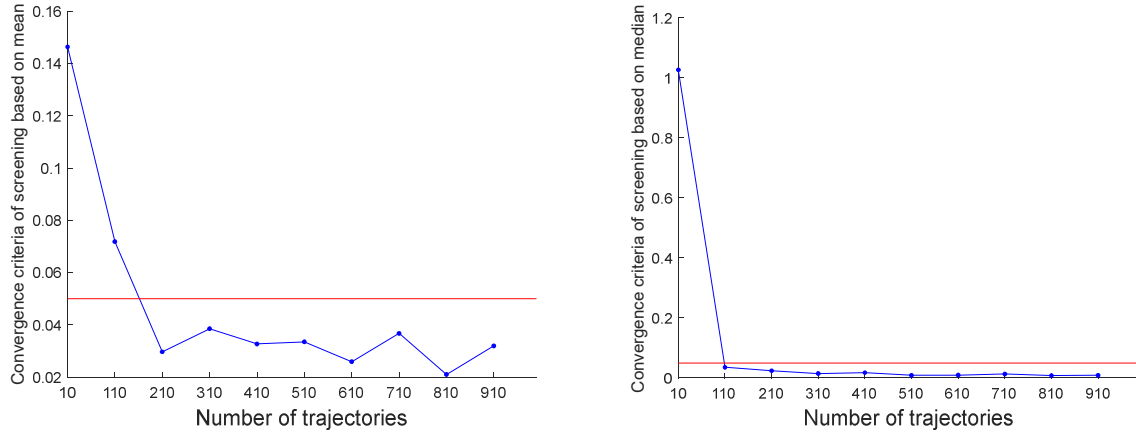


Figure S12 : The calculation of $Stat_{input\ pairs\ screening}$ to assess the screening convergence of the carbonation model input pairs, using the normalized indices based on the mean (a) and based on the median (b) of MEE of the Morris' extension method.

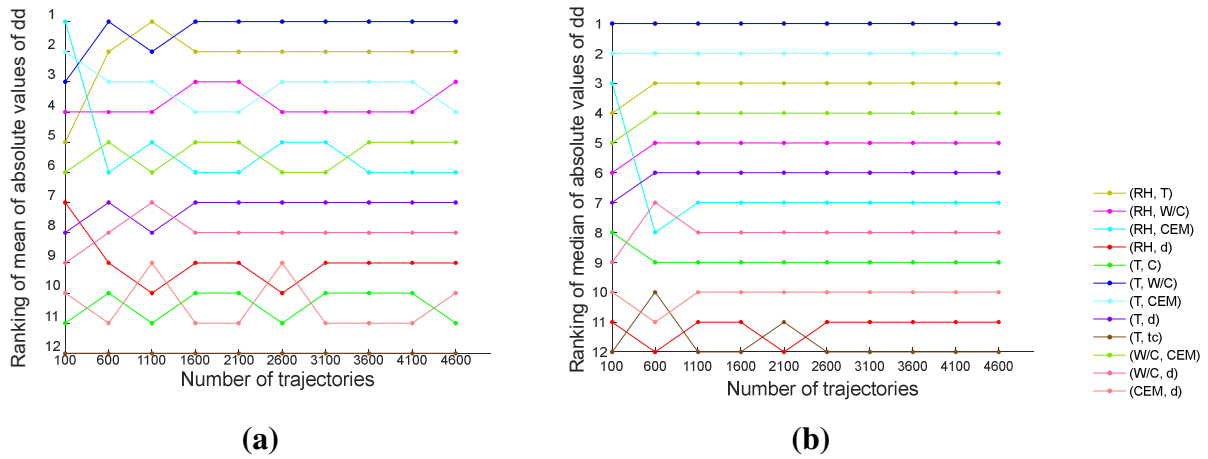
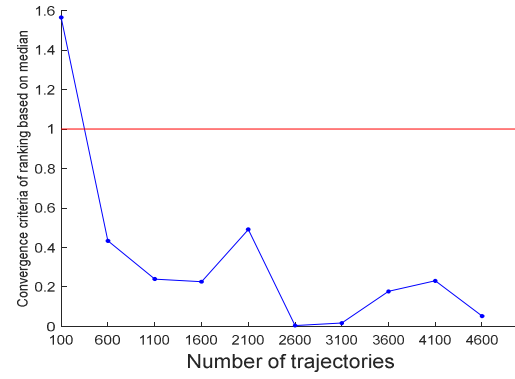
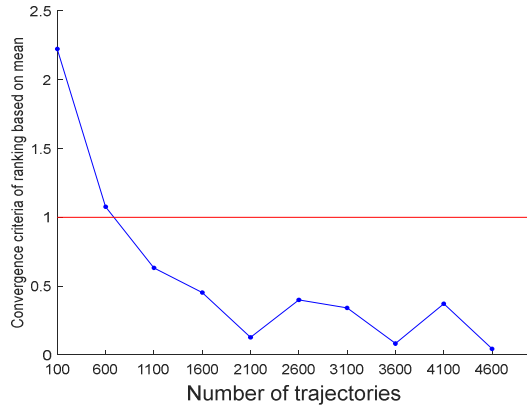


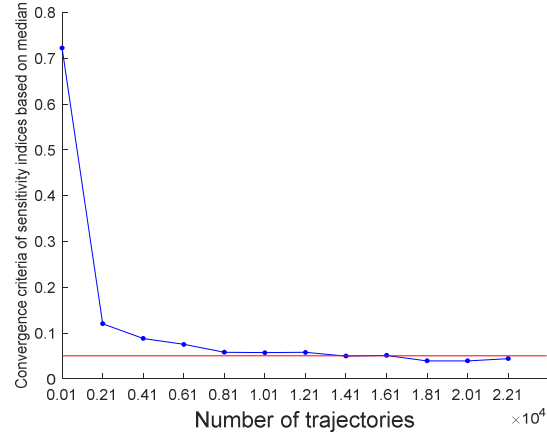
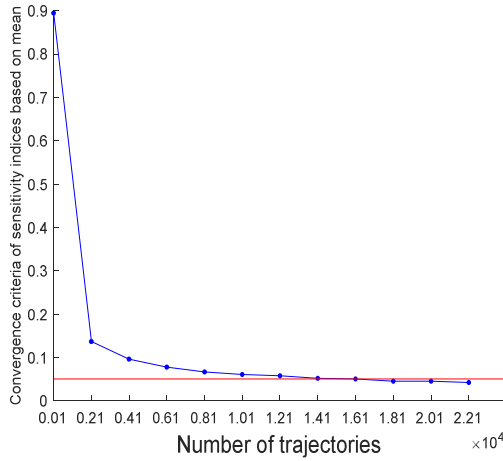
Figure S13 : Ranking of pairs of input parameters of the carbonation model, when using mean (a) and median (b) of absolute values of MEE for the Morris' extension method using the sampling strategy of Handcuffed Prisoners.



(a)

(b)

Figure S14 : The calculation of $Stat_{input\ pairs\ ranking}$ to assess the ranking convergence of the carbonation model input pairs, using the normalized indices based on the mean (a) and based on the median (b) of MEE of the Morris' extension method.



(a)

(b)

Figure S15 : The calculation of $Stat_{input\ pairs\ indices}$ to assess the convergence of sensitivity indices values of the carbonation model input pairs, using the normalized indices based on the mean (a) and based on the median (b) of MEE of the Morris' extension method.

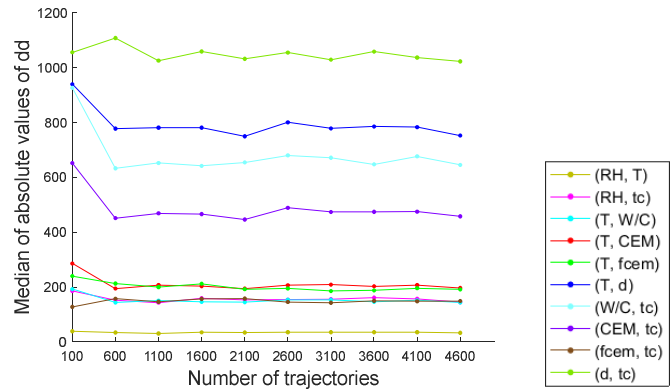
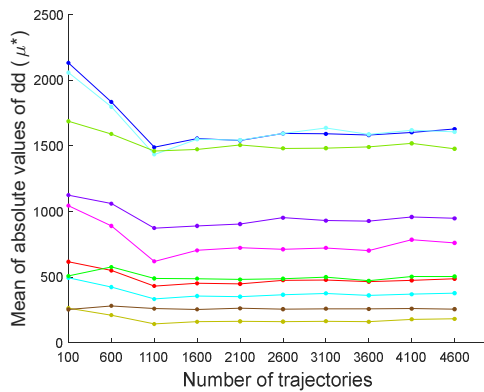


Figure S16 : Indices μ_{ij}^* (a) and γ_{ij}^* (b) of the Morris' extension method using the sampling strategy of cycle equitable graphs.

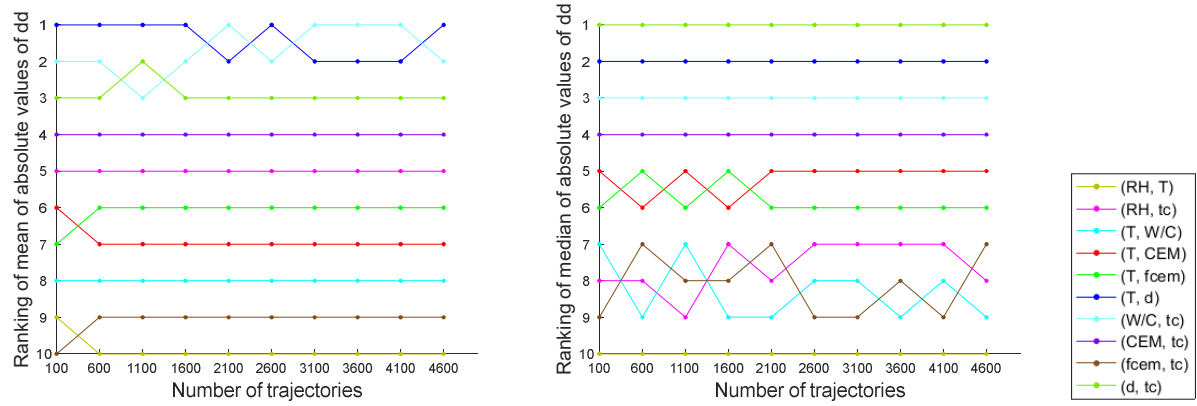


Figure S17 : Ranking of pairs of input parameters of the carbonation model, when using mean (a) and median (b) of absolute values of MEE for the Morris' extension method using the sampling strategy of cycle equitable graphs.

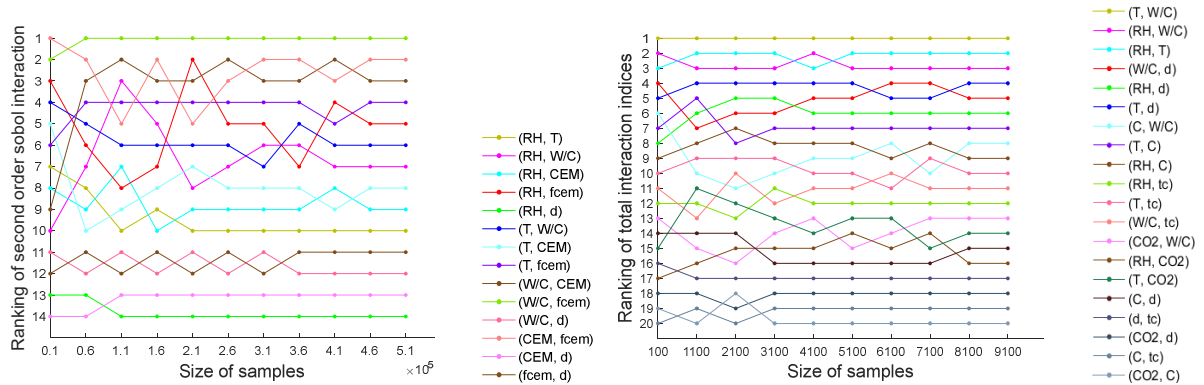


Figure S18 : Ranking of second-order (a) and total interaction (b) Sobol indices of input pairs of the carbonation model according to their combined influences.

	Number of trajectories (r)									
	100	600	1100	1600	2100	2600	3100	3600	4100	4600
Calculation cost of Morris method	1200	7200	13200	19200	25200	31200	37200	43200	49200	55200

Table S11 : The calculation cost according to the number of trajectories used in the application of Morris method to the carbonation model.

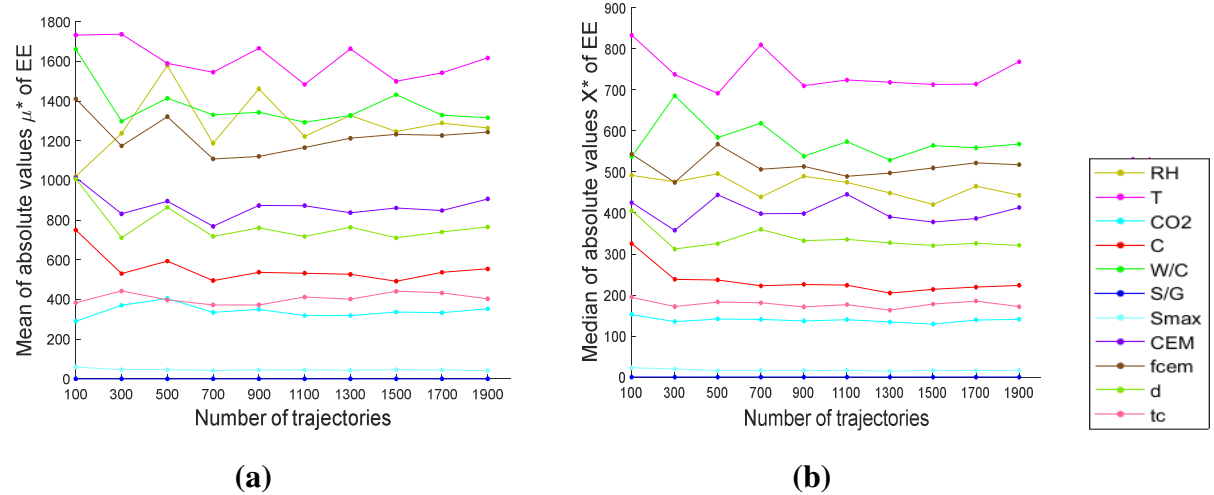


Figure S19 : Variations of the mean (a) and median (b) of absolute values of elementary effects (EE) for input parameters of the carbonation model by applying the Morris method.

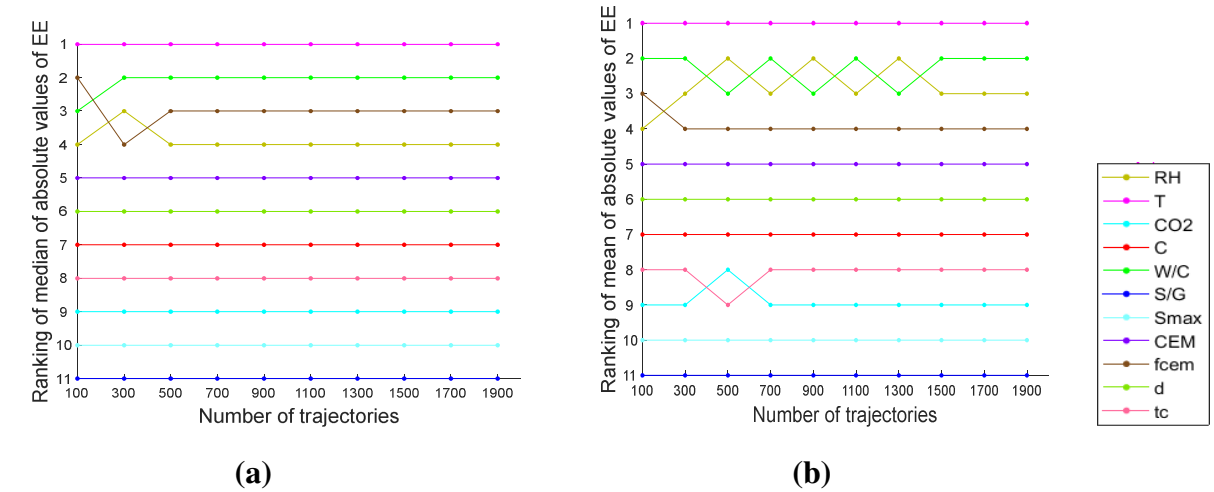


Figure S20 : Ranking of input parameters of the carbonation model, when using mean (a) and median (b) of absolute values of elementary effects (EE) for the Morris method.