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# 1 **Convergence of sensitivity analysis methods for evaluating** 2 **combined influences of model inputs**

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34 ***Abstract***

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

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

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## 64 **1. Introduction**

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

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

85 To address these issues, various SA methods are available in the literature. One group  
86 of methods is considered as local SA methods, which measured the output sensitivity to the  
87 variations of the inputs from their nominal values one at a time (OAT). Local SA used a  
88 sampling strategy in which output variations are calculated by varying one input parameter at a  
89 time, while keeping all others constant [7]. Another group of methods is considered as global  
90 SA methods, which are characterized by the exploration of the entire space of the input  
91 parameters. This includes Morris elementary effects method [8] using OAT sampling strategy  
92 and its extension for the case of mixed effects [9, 10], methods based on linear regression  
93 (standard regression coefficient, linear regression coefficient and partial correlation coefficient)  
94 [11], those based on the derivatives [12, 13] (derivative-based global sensitivity measures,  
95 DGSM [14] and crossed-DGSM [15]) and on the moment independent (PDF and CDF based)  
96 [5, 16, 17], and the methods based on the decomposition of the variance (Sobol indices) [18,  
97 19]. These methods are particularly valuable tools for the development, analysis, and use of

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

104

| SA Methods  | Type  |        |             |              | Order of calculated sensitivity indices |                 |                          |                                      | Identifying the sense of influence |                      | Identifying the shape of influence |                      |            |   |               | Calculation cost (number of model evaluations) |              |                            |
|---|-------|--------|-------------|--------------|---|-----------------|--------------------------|--------------------------------------|------------------------------------|----------------------|------------------------------------|----------------------|------------|---|---------------|--|--------------|----------------------------|
|   | Local | Global | Qualitative | Quantitative | First order                             | Total influence | Second-order interaction | Higher-order interaction (order > 2) | Total interaction                  | Individual influence | Interaction influence              | Individual influence |            | 2 <sup>nd</sup> order 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 ( $\sim 10000$  for Sobol [20] and  $\sim 100$  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 ( $\sim 10$  to  $50$  for Morris method [22] and more for Morris' extension, depending on the complexity degree of model).

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

107

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

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

136

137 SA is frequently required as a method to identify and characterize the relationships of  
138 interacting factors, and their influence on a model response is a crucial issue in many studies.  
139 For instance, in human genetics, the identification of risk loci and their interactions investigated  
140 [24]. Likewise, in medicine, a SA technique is developed for interaction analyses between  
141 biological and chemical exposures, which is a challenge in epidemiologic research and can bias  
142 effect measures [25]. In building energy models, the relative influence of a couple of input  
143 parameters is investigated for developing models that take into account coupling between  
144 phenomena, such as occupancy, micro-climate and building envelope [23, 26]. Particularly, in  
145 the latter study, the Morris' extension method is applied to identify the most influential pairs of  
146 inputs.

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

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

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

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

192

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

198

| <b>Nomenclature abbreviations, symbols and nomenclature</b> |   |
|---|---|
| $\mu$   | Mean of elementary effects                      |
| $\mu^*$   | Mean of absolute values of elementary effects   |
| $\sigma$  | Standard deviation of elementary effects        |
| $\gamma$  | Median of elementary effects                    |
| $\gamma^*$  | 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 <sub>2</sub> | CO <sub>2</sub> -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                     |

199

## 200 2. Sensitivity analysis methods

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

$$205 \quad f : \mathbb{R}^n \rightarrow \mathbb{R}$$

$$206 \quad X \mapsto Y = f(X)$$

207

### 208 2.1. Morris' extension method [9]

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

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

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

219 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

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

220

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

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

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

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

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

$$228 \quad \text{I: } x = (x_1, \dots, x_n); \quad \text{II: } (x + e_i\Delta_i);$$

229

$$230 \quad \text{III: } (x + e_j\Delta_j); \quad \text{IV: } (x + e_i\Delta_i + e_j\Delta_j).$$

231 For a model containing  $n$  input parameters, the number of possible combined-actions of  
 232 two parameters, given by  $\binom{n}{2} = \frac{n(n-1)}{2}$ , defined the number of elements of the set  $T_{ij} =$   
 233  $\{dd_{ij}(x) \mid x \in Q_n\}$ . The sensitivity indices of the Morris' extension method (see later equations  
 234 (4), (5) and (6)) are estimated using the following two sampling strategies  
 235 (experimental plans). The goal of these experimental designs is to extract randomly a sample  
 236 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].

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

241

### 242 **2.1.1. Sampling strategy of “Handcuffed Prisoners”**

243 The "Handcuffed Prisoners" design is used when the number of input parameters is even  
 244 [9], which is a mathematical solution to the graph theory problem, to optimize the number of  
 245 model evaluations needed to evaluate the second order combined-action effects. By analogy  
 246 with the sampling scheme for the simple Morris method [8], the basic idea is to construct a  
 247 multiple trajectory (MT) to estimate the mixed effect  $dd_{ij}$  for all  $\binom{n}{2}$  pairs of input parameters.  
 248 MT is constructed by joining together a set of simple trajectories having all the same starting  
 249 point. MT must retain the properties required by the simple Morris method such that at least  
 250 one elementary effect  $E_i$  per input can be estimated. As in the simple Morris method, each  
 251 simple trajectory in  $Q_n$  corresponds to a simple orientation matrix  $B_i$  such that its elements are  
 252 either 0 or 1. In addition, for each value of  $i = 1, 2, \dots, n$ , there are two rows of  $B_i$  that differ  
 253 only in the  $i^{\text{th}}$  entries. For instance, the simple orientation matrix in  $Q_4$  is given by:

$$254 \quad B_4 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

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

$$258 \quad M_B = \begin{bmatrix} B_1 \\ B_2 \\ \vdots \\ B_t \end{bmatrix}, \text{ of dimension } (\sum_{i=1}^t m_i) - \text{by} - n.$$

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

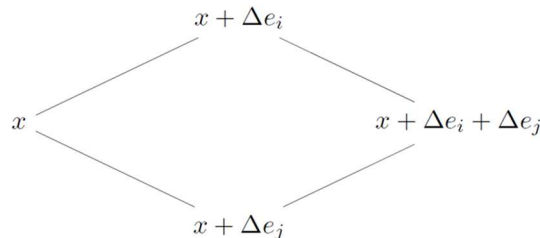
264 second-order elementary effect  $EE_{n-1}$  for the pair of inputs  $(X_{n-1}, X_n)$ , it must use the  
 265 difference of the values of the function  $f$  for the coordinates of  $(n+1)^{th}$  and  $(n-1)^{th}$  rows  
 266 of the matrix  $B$ . Each path defines a simple orientation matrix  $B$  or a simple Morris trajectory,  
 267 which means that the multiple trajectory is constructed from multiple paths. Each path allows  
 268 the computation of all second order elementary effects for all pairs of two successive points of  
 269 this path. In a path, for each input parameter, the combined-actions that are taken into account  
 270 are with the preceding parameter and the next parameter according to this path. Thus, the  
 271 objective is to: “Find a partition of  $\Gamma$  made of  $\frac{n}{2} (= s)$  subsets such that each of this subset is  
 272 composed of  $(n-1)$  handcuffed pairs”. These  $(n-1)$  handcuffed pairs  $\{(i_1, i_2),$   
 273  $(i_2, i_3), \dots, (i_{n-1}, i_n)\}$  represents a path designated by  $\langle i_1, i_2, \dots, i_n \rangle$ , for  $n$  being even ( $n = 2s$ ).  
 274 Finally, in order for a handcuffed design to exist, the following conditions must be satisfied  
 275 [34]:

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

279  
 280 More details have been stated in this case and the case where the number of input parameters  
 281 of a model  $n$  is odd ( $n = 2s + 1$ ) [9].

### 282 283 2.1.2. Sampling strategy of “cycle equitable graphs”

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



287  
 288 **Figure 1:** The form of a quadratic cycle [10].

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

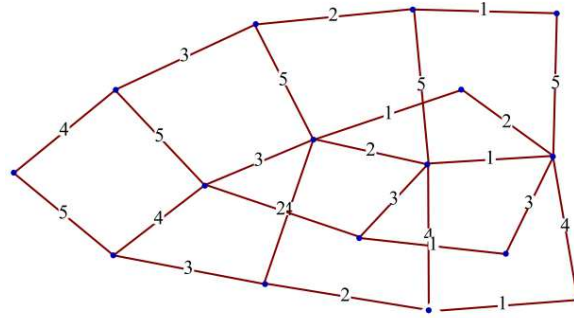
291 Let  $S \subset Q_n$  denote the subgraphs of the unit hypercube with dimension  $n : Q_n = [0,1]^n$   
 292 (where  $n$  is the number of input parameters of a model).

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

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

300

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



303

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

305

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

309

### 310 2.1.3. Sensitivity indices

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

- 313 • the mean of MEE :

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

- 314 • 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  $\mu_{ij}^*$  of values  $dd_{ij}$  is a measure of the relative  
 319 importance of the combined-actions of two input parameters, while  $\sigma_{\mu}$  (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  $\geq 3$ . Thus, using  $\mu_{ij}^*$  and  $\sigma_{\mu}$   
 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  $\mu_{ij}^*$  and  $\sigma_{\mu}$  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  $\mu_{ij}^*$  is high and  $\sigma_{\mu}$  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  $\sigma_{\mu}$  is high (independently of the value of  $\mu_{ij}^*$ ), 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:

$$337 \quad dd_{ij}(x) = \frac{f(x + e_i\Delta_i + e_j\Delta_j) - f(x + e_i\Delta_i) - f(x + e_j\Delta_j) + f(x)}{\Delta_i\Delta_j}$$

$$338 \quad = \frac{f(x_i + \Delta_i, x_j + \Delta_j) - f(x_i + \Delta_i, x_j) - f(x_i, x_j + \Delta_j) + f(x_i, x_j)}{\Delta_i\Delta_j}$$

$$339 \quad = \frac{a(x_i + \Delta_i) + b(x_j + \Delta_j) + c(x_i + \Delta_i)(x_j + \Delta_j) - [a(x_i + \Delta_i) + bx_j + c(x_i + \Delta_i)x_j]}{\Delta_i \Delta_j}$$

$$340 \quad - \frac{[ax_i + b(x_j + \Delta_j) + cx_i(x_j + \Delta_j)] + ax_i + bx_j + cx_ix_j}{\Delta_i \Delta_j}$$

$$341 \quad = \frac{c\Delta_i \Delta_j}{\Delta_i \Delta_j} = c = \text{constant.}$$

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

$$343 \quad \mu_{ij} = \frac{1}{r} \sum_{l=1}^r dd_{ij}^{(l)} = \frac{r \times c}{r} = c = \text{constant} = \mu_{ij}^*.$$

$$344 \quad \sigma_\mu = \sqrt{\frac{1}{r} \sum_{l=1}^r (dd_{ij}^{(l)} - \mu_{ij})^2} = \frac{1}{r} \sqrt{\sum_{j=1}^r [c - c]^2} = 0.$$

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

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

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

370 Note that the ratio  $\sigma_\mu/\mu_{ij}^*$  is another measure suggested for the classification of the combined-  
 371 actions influence of the pair of inputs  $(X_i, X_j)$  on the output (for more details, see **Section III**  
 372 in Supplementary Material).

373

### 3742.2. Sobol method

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

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

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

382

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

383 where

$$384 \quad V_i = V(E[Y | X_i]),$$

$$385 \quad V_{ij} = V(E[Y | X_i, X_j]) - V_i - V_j,$$

$$386 \quad V_{ijk} = V(E[Y | X_i, X_j, X_k]) - V_{ij} - V_{ik} - V_{jk} - V_i - V_j - V_k,$$

387 and so on until order  $n$ .

388

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



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

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

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

392 and so on until order  $n$ .

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

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

396 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  $Y = f$   
 397  $(X_1, X_2, X_3, X_4)$ , the superset importance  $S_{1,2}^{super} = S_{12} + S_{123} + S_{124} + S_{1234}$ .

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

410

### 411 2.3. Convergence criteria

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

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

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

421

422 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  $\mu_{ij}^*$  and  $\gamma_{ij}^*$ , respectively, for  
 423 all input pairs possible  $(X_i, X_j)$ . These normalized indices still provide semi-quantitative  
 424 measures of sensitivity. For the second-order and total interaction indices of Sobol, we  
 425 considered  $SI_{ij} = S_{ij}$  and  $SI_{ij} = S_{ij}^{Super}$ , respectively.

426

### 427 **2.3.1. Convergence of the sensitivity indices value**

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

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

433 where  $SI_{ij}^{ub}$  and  $SI_{ij}^{lb}$  are the upper and lower bounds of the normalized sensitivity index  $SI_{ij}$  of  
 434  $(X_i, X_j)$ , with  $n$  being the number of model input parameters. The convergence of sensitivity  
 435 indices value is considered to be reached when the value of  $Stat_{input\ pairs\ indices}$  is lower than  
 436 0.05 [32].

### 437 **2.3.2. Convergence of input pair ranking**

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

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

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

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

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

### 453 2.3.3. Convergence of input pair screening

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

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

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

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

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

463

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

466

### 467 3. Applications and Results

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

475

#### 476 3.1. Theoretical model

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

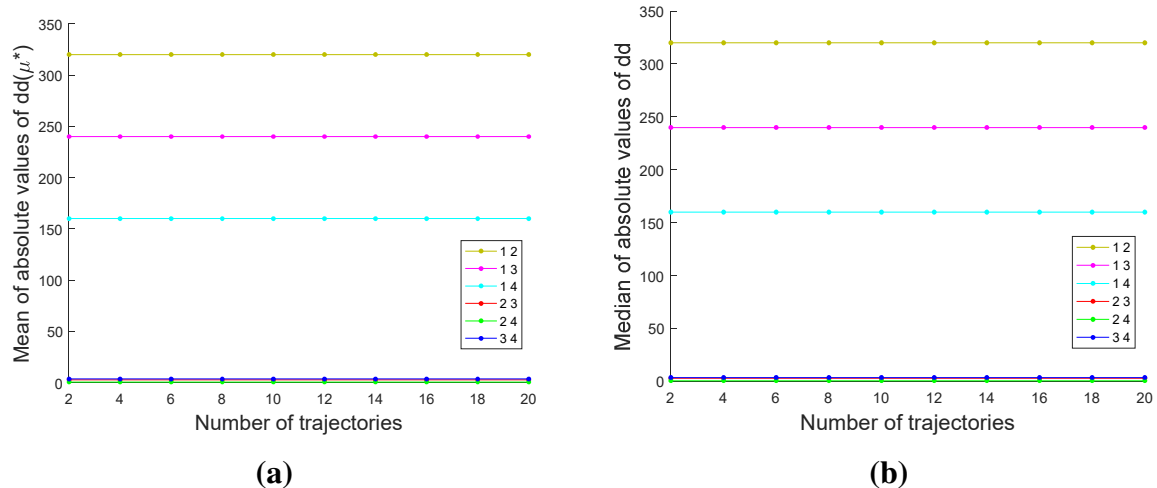
$$f = \sum_{i=1}^4 b_i w_i + \sum_{i \leq j} b_{ij} w_i w_j \quad (17)$$

478 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  
479 the following standard values:  $b_3 = 10$ ;  $b_{22} = 30$ ;  $b_{12} = 80$ ;  $b_{13} = 60$ ;  $b_{14} = 40$ . All the other  
480 coefficients are taken to be the absolute values of a set of random numbers generated from a  
481 normal distribution with zero mean and unit standard deviation. In particular, their values are:  
482  $b_1 = 0.05$ ;  $b_2 = 0.59$ ;  $b_4 = 0.21$ ;  $b_{11} = 0.00$ ;  $b_{23} = 0.73$ ;  $b_{24} = 0.18$ ;  $b_{33} = 0.64$ ;  $b_{34} =$   
483  $0.93$ ;  $b_{44} = 0.06$ . The Morris' extension method is applied by incrementally increasing the  
484 number of trajectories ( $r$ ) from 2 to 20 (**Figure 3**), and Sobol method (second-order and total  
485 interaction) runs by incrementally increasing the size of classical Monte-Carlo samples ( $N$ )  
486 from 100 to 5600 (**Figure S11** in Supplementary Material).

487

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

495



496  
497

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

501

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

512

| 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    | $(X_1, X_4)$                  | $(X_1, X_4)$ | $(X_1, X_4)$             | $(X_1, X_4)$ | $(X_1, X_4)$               | $(X_1, X_4)$              |

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

516

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

522

|  | 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 |

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

525

|  | 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 |

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

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

530

### 531 3.2. Case study: concrete carbonation model

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

$$x_{CO_2} = A \cdot \sqrt{t} \tag{18}$$

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

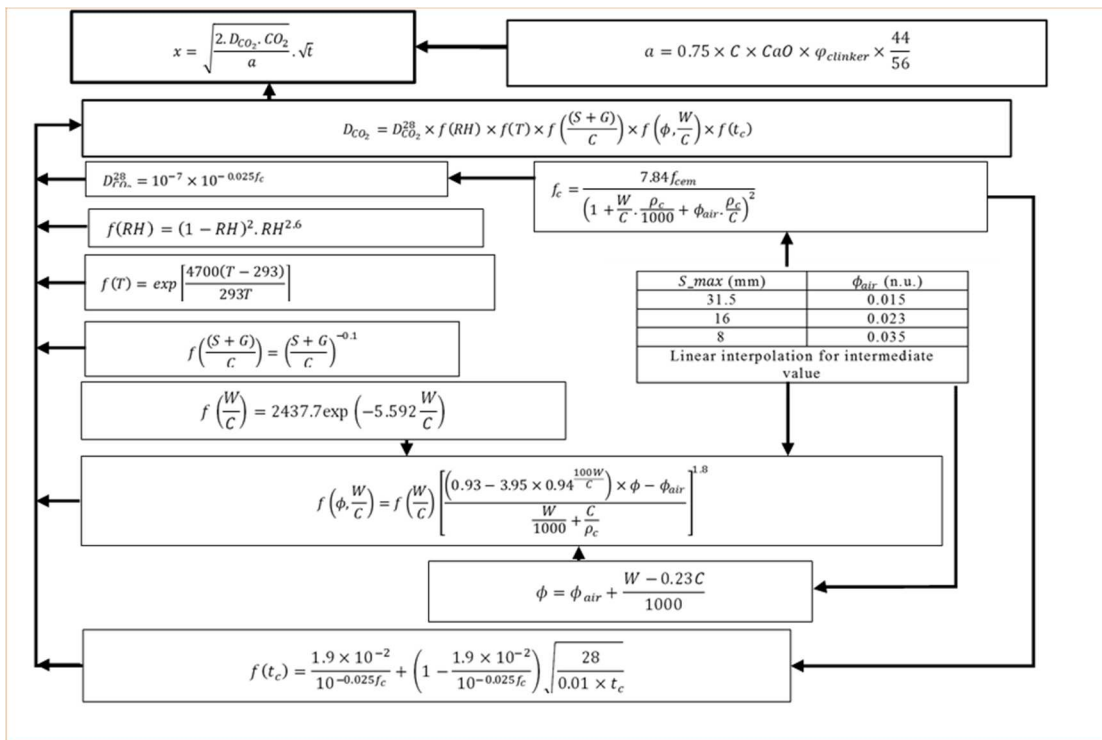
$$A = f(RH, T, CO_2, C, W/C, S/G, S_{max}, CEM, f_{cem}, t_c) = \sqrt{\frac{2 \cdot D_{CO_2} \cdot [CO_2]_{ext}}{a}} \quad (19)$$

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

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

545  
 546 Ta et al. [33] used this model to identify the individual effects of the input parameters  
 547 on the corrosion initiation time, by using simple Morris method and Sobol SA method.  
 548 However, non-negligible effects of combined-actions of inputs of carbonation model were  
 549 pointed out on the corrosion initiation time but still remain to be studied. Summary descriptive  
 550 statistics (mean, min: minimum, max: maximum, COV: the variation coefficient) and the  
 551 probability distribution of the input parameters are given in the **Table 5**.

552



553

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

555

| 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 <sup>3</sup> | 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 <sub>2</sub>  | Ppm               | 380   | 304,5<br>6 | 456,8 | 0,05 | Truncated Normal                     |

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

557

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

567

### 568 3.2.1. Results of Morris' extension method

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

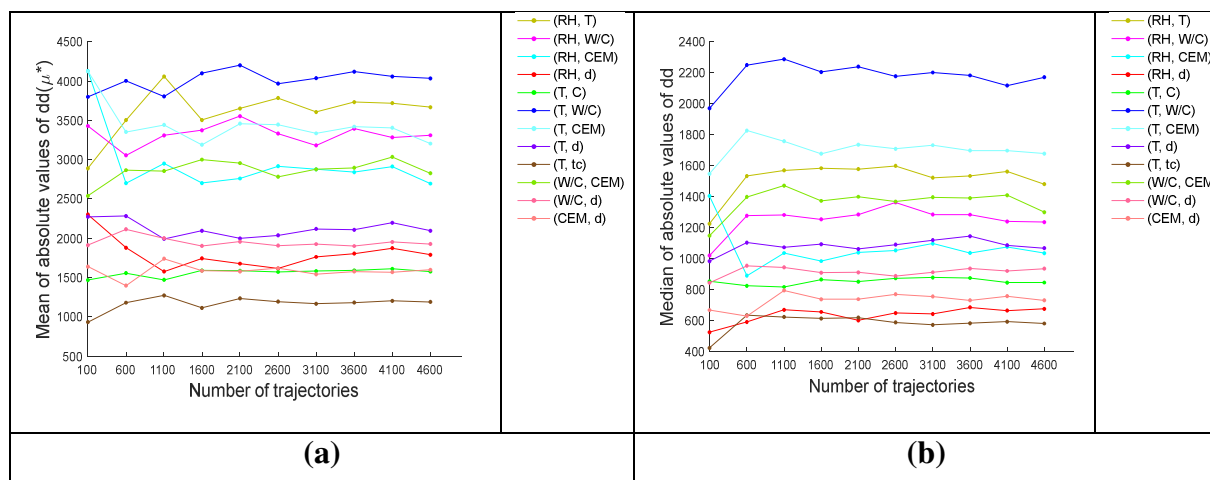


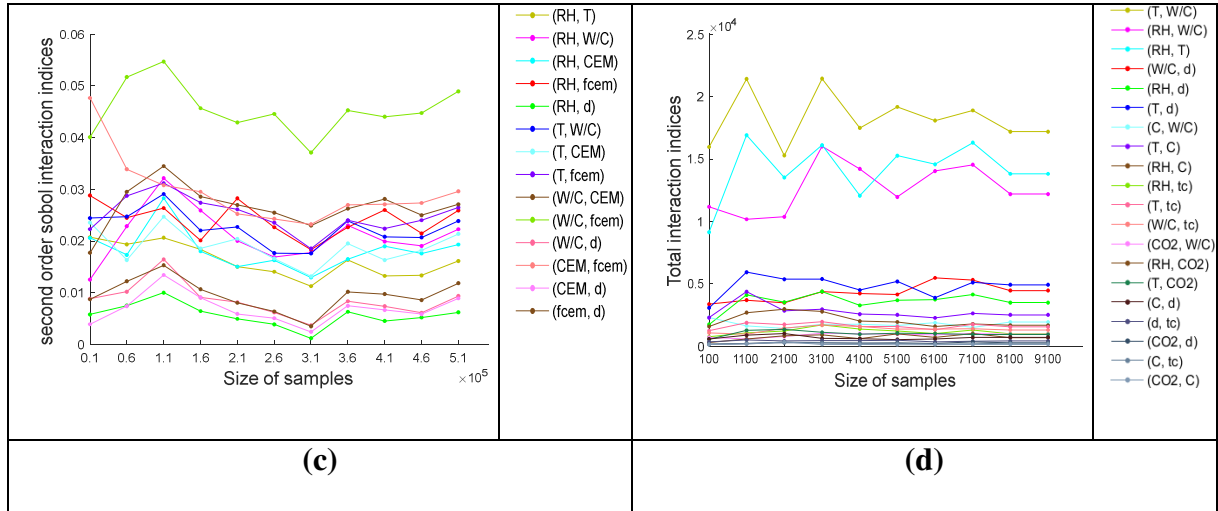
571 based on the sampling strategy of Handcuffed Prisoners on the carbonation model. The  
 572 magnitude of indices based on the mean of MEE enables to quickly distinguish influential and  
 573 non-influential groups of input pairs of carbonation model, from the minimum number of  
 574 trajectories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

577 The criteria in Section 2.3 were implemented to assess the three types of convergence.  
 578 The convergence of screening results of input pairs was achieved from 110 and 150 trajectories  
 579 when using indices  $\gamma_{ij}^*$  and  $\mu_{ij}^*$  based on median and mean of MEE, respectively (**Figure S12**  
 580 in Supplementary Material). Then, the convergence of ranking results was achieved from  
 581 around 2,600 trajectories with indices  $\gamma_{ij}^*$  based on the median of MEE, whereas more than  
 582 4,600 were required to achieve this convergence with indices  $\mu_{ij}^*$  based on the mean of MEE  
 583 (**Figure S13** and **Figure S14** in Supplementary Material). The influential pairs of inputs were  
 584 globally the same using the indices based on the mean and median of MEE but with little  
 585 changes in their relative ranking (**Table 6**). The convergence of values of indices  $\gamma_{ij}^*$  and  $\mu_{ij}^*$   
 586 was achieved from a similar number of 14100 trajectories (**Figure S15** in Supplementary  
 587 Material).

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

593





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

597

| 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)                   |

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

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

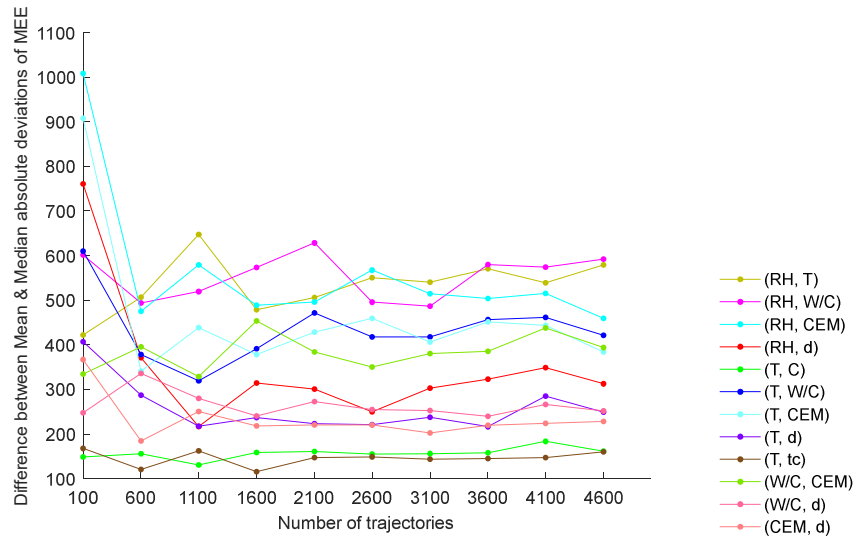
|                                |
|--------------------------------|
| Number of trajectories ( $r$ ) |
|--------------------------------|

|  | 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 |

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

611

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



616

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

619

### 620 3.2.2. Results of second-order and total interaction Sobol indices

621 Concerning the two indices based on variance decomposition of model output, the  
622 magnitude of total interaction indices enabled to distinguish influential and non-influential  
623 groups of pairs of inputs from the minimum number of samples considered (herein, equal to  
624 100, **Figure 5(d)**). Comparatively, the magnitude of second-order Sobol indices pointed out the  
625 most influential pair of inputs (**Figure 5(c)**). The ranking of the first third most influential pairs  
626 of inputs was achieved through convergent sensitivity indices with a smaller sample size  
627 (herein, 5,100) for total interaction sensitivity indices than for second-order indices (herein,  
628 460,000) (**Figure S18** in Supplementary material). Likewise, to achieve the convergence of  
629 total interaction sensitivity indices would require a smaller sample size than second order

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

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

642

|  | 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 |
|  |                     |        |         |         |         | 0       | 0       | 0       | 0       | 0       |         |

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

645

|  | 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 |

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

648

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

651

## 652 4. Discussions and interpretations

### 653 4.1. Convergence of combined influences results

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

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

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

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

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

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

712 In our study, for the application of Morris' extension method on the carbonation model, a  
713 number of trajectories  $r = 110$  was sufficient to reach the convergence of input pairs screening,  
714 while  $r = 2600$  and  $r = 14100$  were sufficient to obtain convergent results of input pairs  
715 ranking and sensitivity indices values, respectively. However, for the application of Sobol  
716 method on the carbonation model, when using the total interaction indices a sample size  $N =$   
717 100 was sufficient to reach the convergence of input pairs screening but the ranking of the third  
718 most influential pairs was achieved from  $N = 5600$ , while  $N = 8100$  was sufficient to obtain  
719 convergent results of values of sensitivity indices. Moreover, a sample size  $N = 460,000$  was  
720 sufficient to achieve the convergence of input pairs ranking when using the second-order Sobol  
721 indices.

722

## 723 4.2. Recommendations

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

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

739 The sensitivity indices of Morris' extension method and the total interaction Sobol  
740 indices gave the same results of the total combined influence of input pairs on the model  
741 response. However, to apply Sobol method is more costly than the Morris' extension method.  
742 Thus, the choice between applying these two methods depends on the main researched  
743 information between screening, ranking and quantification of sensitivity indices of input pairs.  
744

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

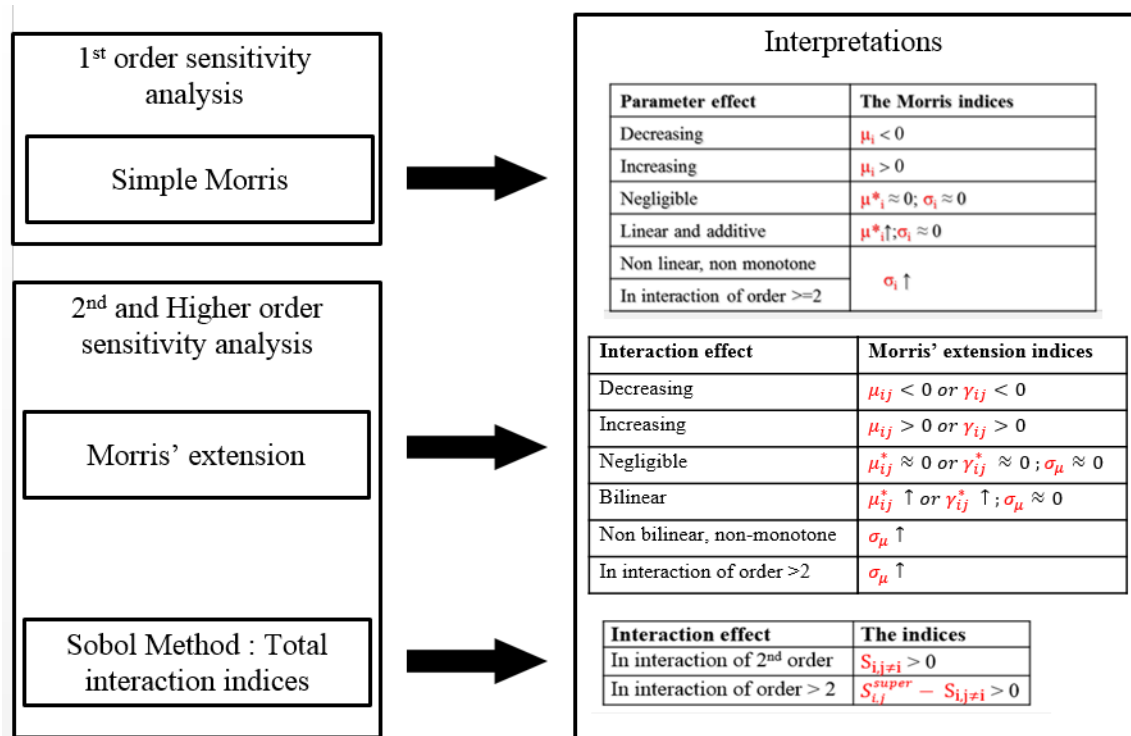
750 (2) The calculation cost of the application of second-order Sobol indices on complex model is  
751 expensive compared with other methods such as the extension of Morris method and the  
752 computation of total interaction indices. Therefore, in order to identify the pairs that have the  
753 more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

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

771

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





781

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

784

## 785 5. Conclusions

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

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

809

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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

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

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

975 This method is based on the discretization of each input variable to obtain  $p$  levels (values)  
 976 between 0 and 1, i.e. it may take as a value  $\{0, 1/(p-1), 2/(p-1), \dots, 1\}$ . Each input parameter  
 977 is assumed to have a uniform distribution  $[0, 1]$  and therefore the space of input parameters  $Q_n$   
 978 is a unit hypercube of dimension  $n$  ( $n$  being the number of input parameters). If an input  
 979 parameter  $X_i$  has a uniform distribution in  $[x_{min}(i), x_{max}(i)]$ , it should to transform this input  
 980 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  
 981 minimum, the maximum and the value of the input parameter  $X_i$ , respectively). We define in  
 982 the hypercube  $Q_n$  a trajectory as a set of  $(n + 1)$  successive points. Each point differs from the  
 983 preceding one only by a single coordinate, such that each component is changed only once by  
 984 a value  $\Delta = p/2(p-1)$ , then the elementary effect of the input parameter  $X_i$  is defined by:

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

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

987 The mean

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

988

989 And the standard deviation

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

990

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

993

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

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

999

## 1000 II. Distinction of linear and non-linear effects for Morris method

1001

1002 We now briefly describe why the sensitivity indices of simple Morris method enable to  
 1003 distinguish linear and non-linear effects on the model output. For instance, consider the input  $X_i$   
 1004 with a linear individual effect on the model output  $Y = f(X) = aX_i + b$ .

1005 For a given value  $x = x_i$  of the input vector, the simple elementary effect of  $X_i$  is given by:

$$1006 E_i(x) = E_i(x_i) = \frac{f(x_i + \Delta) - f(x_i)}{\Delta} = \frac{a(x_i + \Delta) + b - ax_i - b}{\Delta} = \frac{a(\Delta)}{\Delta} = a = \text{constant}.$$

1007 That results in the following respective values of mean and standard deviation of simple  
 1008 elementary effects:

1009

$$1010 \mu_i = \frac{1}{r} \sum_{j=1}^r E_i(x_i^j) = \frac{r \times a}{r} = a = \text{constant} = \mu_i^*$$

$$1011 \sigma_i = \sqrt{\frac{1}{r} \sum_{j=1}^r [E_i(x_i^j) - \mu_i]^2} = \frac{1}{r} \sqrt{\sum_{j=1}^r [a - a]^2} = 0.$$

1012 Thus, firstly, for an input of class (1) with values of  $\mu_i^*$  and  $\sigma_i$  close to zero (i.e.  $a \simeq 0$ ), we  
 1013 have  $Y = f(X) \simeq b$ , which corresponds to the negligible effect of  $X_i$  on model output  $Y$ .

1014 Secondly, for an input of class (2) with the high value of  $\mu_i^*$  (i.e.  $\mu_i^* \gg 0$ ) and low value of  $\sigma_i$ ,  
 1015 we have a non-negligible contribution of the term  $aX_i$  to model output  $Y$  that corresponds to a

1016 linear effect of  $X_i$ . Thirdly, for an input of class (3), the high value of  $\sigma_i \gg 0$  indicates values  
 1017 of  $E_i(x)$  that are not constant. Thus, the parameter  $a$  is not constant and can be assumed to be

1018 a second variable  $a = X_j$ , which implies combined-actions of order  $\geq 2$  of inputs  $(X_i, X_j)$  on  
 1019 model output  $Y$ .

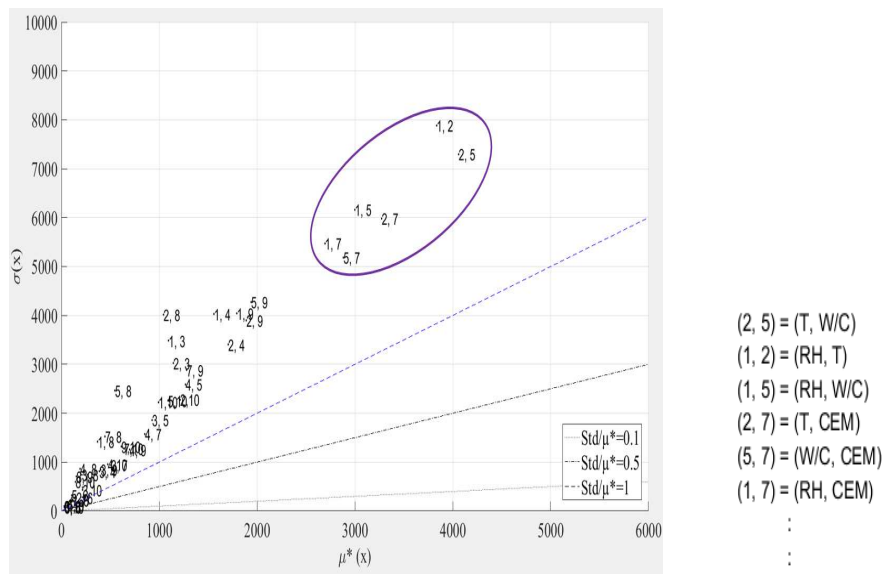
1020

1021 **III. Another measure of Morris' extension method**

1022 The mean  $\mu_{ij}^*$  of absolute values of MEE was introduced above as a measure of importance  
 1023 (combined influence) for the input pair  $(X_i, X_j)$ . This information can be complemented by the  
 1024 ratio  $\sigma_\mu/\mu_{ij}^*$  as an indicator of the shape of combined influence for all possible pairs, i.e. bilinear  
 1025 or non-bilinear effects, as justified below:

- 1026 • 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  
 1027 bilinear or quasi-bilinear effect.
- 1028 • If  $0.1 < \sigma_\mu/\mu_{ij}^* < 0.5$ , we consider that the pair of inputs  $(X_i, X_j)$  has a monotonic effect.
- 1029 • If  $0.5 < \sigma_\mu/\mu_{ij}^* < 1$ , we consider that the pair of inputs  $(X_i, X_j)$  has an almost monotonic  
 1030 effect.
- 1031 • If  $\sigma_\mu/\mu_{ij}^* > 1$ , we consider that the pair of inputs  $(X_i, X_j)$  has non-bilinear effect and / or  
 1032 combined-actions of order  $> 2$  with the other input parameters.

1033



1034

1035 **Figure S8** : The calculation of the ratio  $\sigma_\mu/\mu_{ij}^*$  of Morris' extension method for all possible  
 1036 input pairs of the carbonation model.

1037

1038 Note that the ratio  $\sigma_\mu/\mu_{ij}^*$  was more than 1 for all possible influential pairs of inputs of the  
 1039 carbonation model such that these pairs had a non-bilinear effect and / or combined-actions of  
 1040 order  $> 2$  with the other input parameters (**Figure S8**). In this figure, we applied the Morris'  
 1041 extension method with number of trajectories  $r = 150$ , because from this number we could



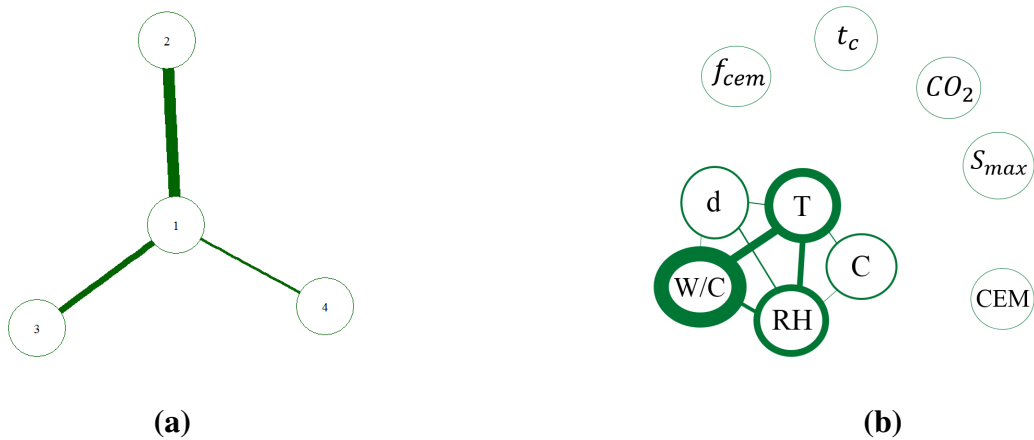
1042 screening out the input pairs that have most influential combined-actions on the carbonation  
1043 model.

1044

#### 1045 **IV. FANOVA graph**

1046 The FANOVA graph is a nice way to visualize the estimated interaction structure. In this graph,  
1047 each vertex represents one input parameter and an edge between two vertices indicates the  
1048 presence of second or higher-order interactions between the input parameters. The thickness of  
1049 the edges is proportional to the total interaction index (TII) and in addition, the thickness of the  
1050 circles around vertices indicates the first-order indices. The early inactive inputs can be detected  
1051 as single thin vertices. The FANOVA graph is intended as a tool supporting structural kernel  
1052 design in the context of non-parametric modelling using Gaussian processes (kriging), whose  
1053 complexity and performance can improve if the kernel's structure closely reflects the clique  
1054 structure of the FANOVA graph. Being based on Sobol indices, the set of total variation indices  
1055 that the FANOVA graph describes are computed by Monte Carlo techniques, and thus they  
1056 inherit the complexity of Sobol indices.

1057 The two FANOVA graphs of our models are shown below (**Figure S9**).



1058

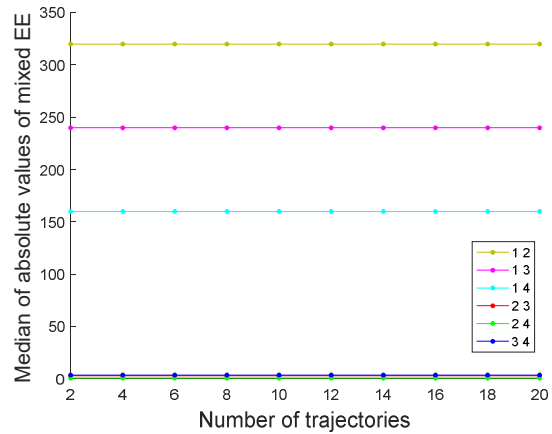
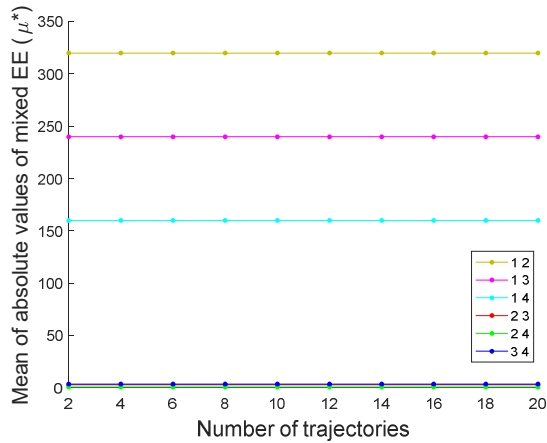
1059

1060 **Figure S9** : (a) and (b) are the FANOVA graphs of the theoretical and carbonation models,  
1061 respectively.

1062

#### 1063 **V. Additional graphs and tables**

1064



1065

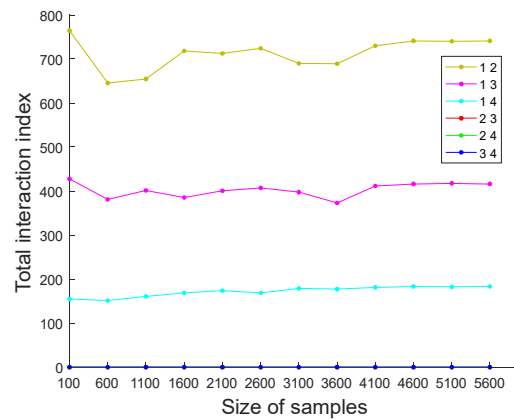
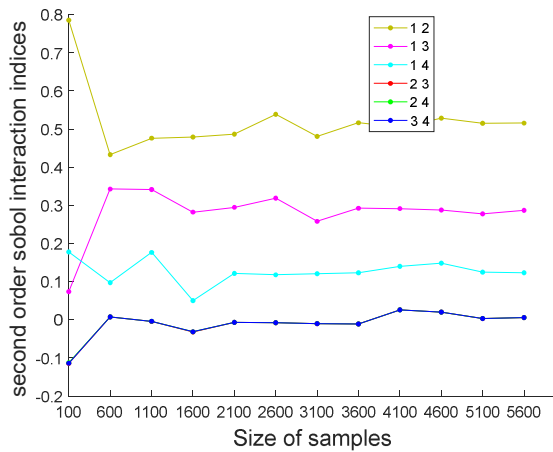
(a)

(b)

1066

1067 **Figure S10** : Variations of the mean (a) and median (b) of absolute values of MEE for pairs of  
 1068 input parameters of the theoretical model by applying the Morris' extension method using the  
 1069 sampling strategy of cycle equitable graphs [10].

1070



1071

(a)

(b)

1072

1073 **Figure S11** : Variations of the second-order (a) and total (b) interaction Sobol indices of pairs  
 1074 of input parameters of the theoretical model.

1075

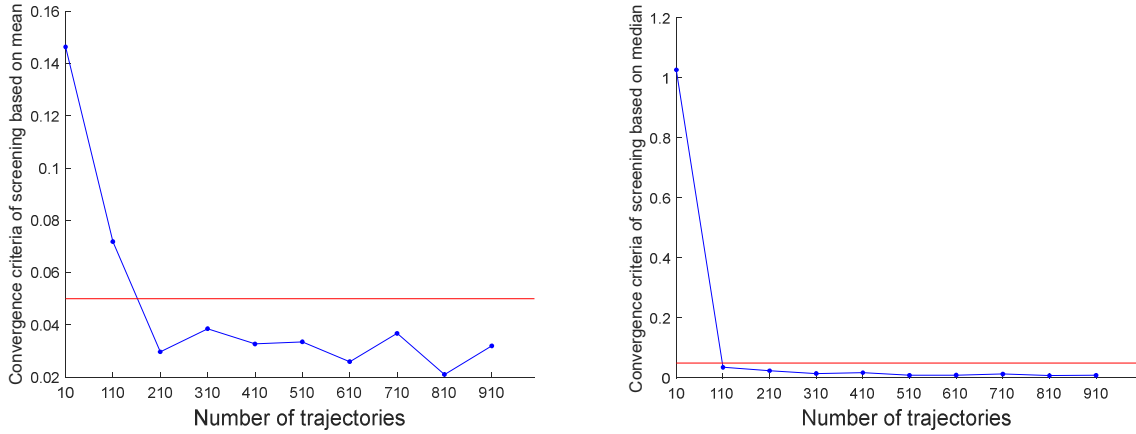
1076

| $r$        | 100  | 600 | 1100 | 1600 | 2100 | 2600 | 3100 | 3600 | 4100 | 4600 |
|------------|------|-----|------|------|------|------|------|------|------|------|
| (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  |

1077

1078 **Table S10:** The values of the difference ( $E_{\mu^*} - E_{\gamma^*}$ ) of mixed elementary effects (MEE) of the  
 1079 most influential pairs of inputs on the carbonation model.

1080



1081

(a)

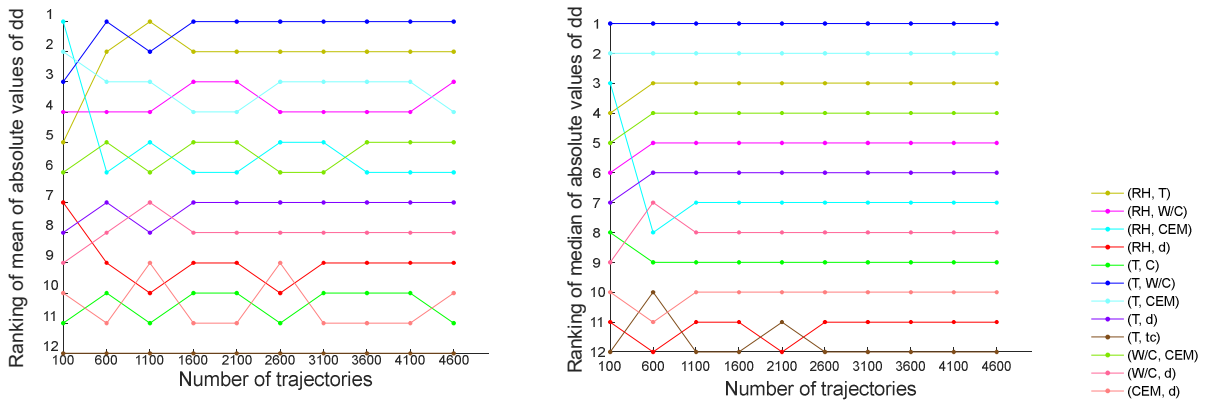
(b)

1082

1083 **Figure S12 :** The calculation of  $Stat_{input\ pairs\ screening}$  to assess the screening convergence of  
 1084 the carbonation model input pairs, using the normalized indices based on the mean (a) and  
 1085 based on the median (b) of MEE of the Morris' extension method.

1086

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1088

(a)

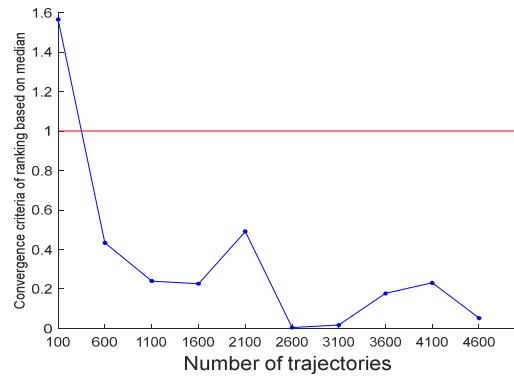
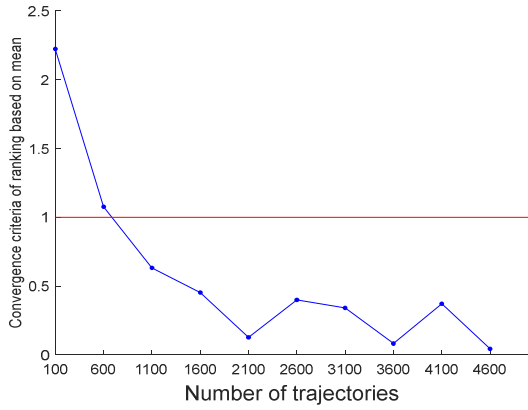
(b)

1089

1090 **Figure S13 :** Ranking of pairs of input parameters of the carbonation model, when using mean  
 1091 (a) and median (b) of absolute values of MEE for the Morris' extension method using the  
 1092 sampling strategy of Handcuffed Prisoners.

1093

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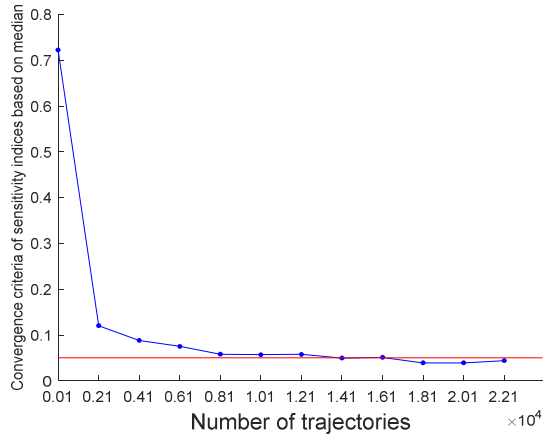
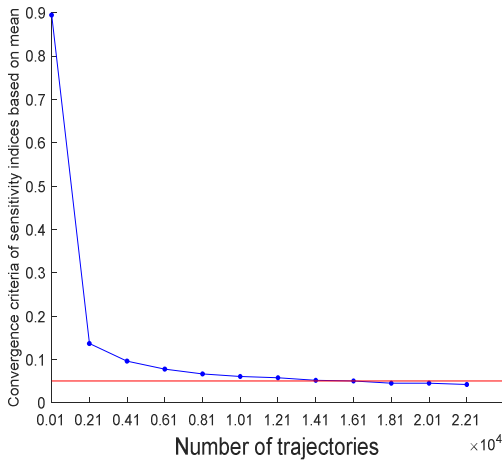
1095

1096

(a)

(b)

1097 **Figure S14 :** The calculation of  $Stat_{input\ pairs\ ranking}$  to assess the ranking convergence of  
 1098 the carbonation model input pairs, using the normalized indices based on the mean (a) and  
 1099 based on the median (b) of MEE of the Morris' extension method.



1100

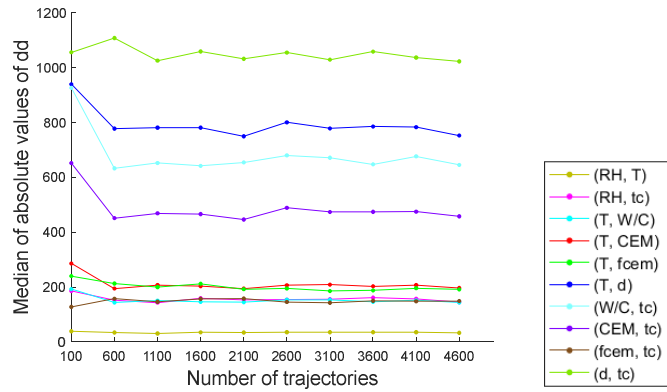
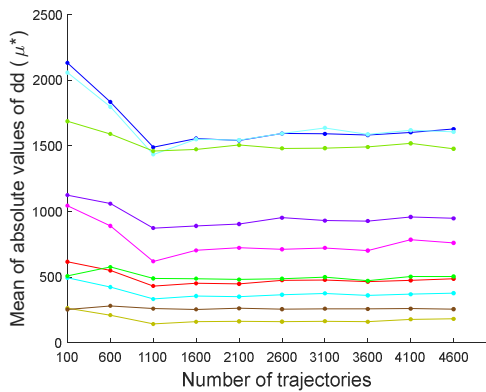
1101

(a)

(b)

1102 **Figure S15 :** The calculation of  $Stat_{input\ pairs\ indices}$  to assess the convergence of sensitivity  
 1103 indices values of the carbonation model input pairs, using the normalized indices based on the  
 1104 mean (a) and based on the median (b) of MEE of the Morris' extension method.

1105



1106

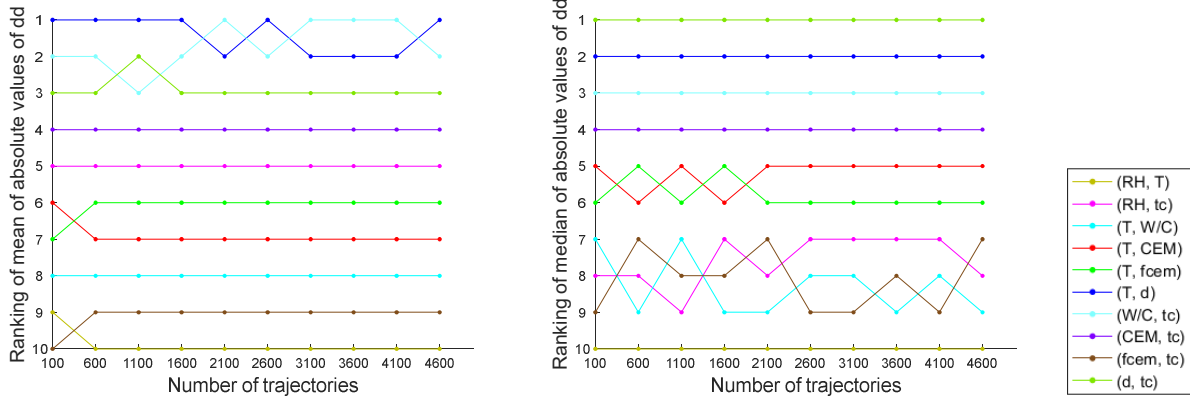
1107

(a)

(b)

1108 **Figure S16** : Indices  $\mu_{ij}^*$  (a) and  $\gamma_{ij}^*$  (b) of the Morris' extension method using the sampling  
 1109 strategy of cycle equitable graphs.

1110



1111

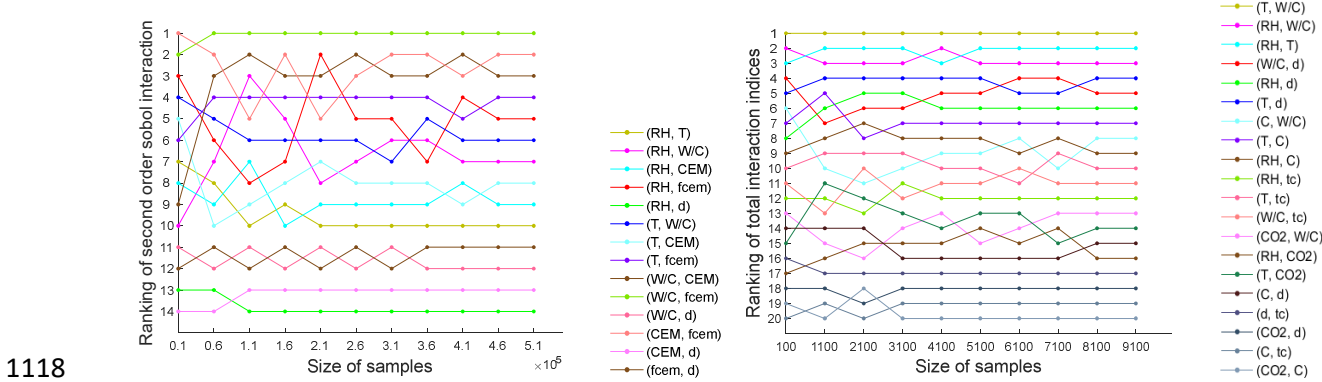
(a)

(b)

1112 **Figure S17** : Ranking of pairs of input parameters of the carbonation model, when using mean  
 1113 (a) and median (b) of absolute values of MEE for the Morris' extension method using the  
 1114 sampling strategy of cycle equitable graphs.

1115

1116



1117

(a)

(b)

1118 **Figure S18** : Ranking of second-order (a) and total interaction (b) Sobol indices of input pairs  
 1119 of the carbonation model according to their combined influences.

1120

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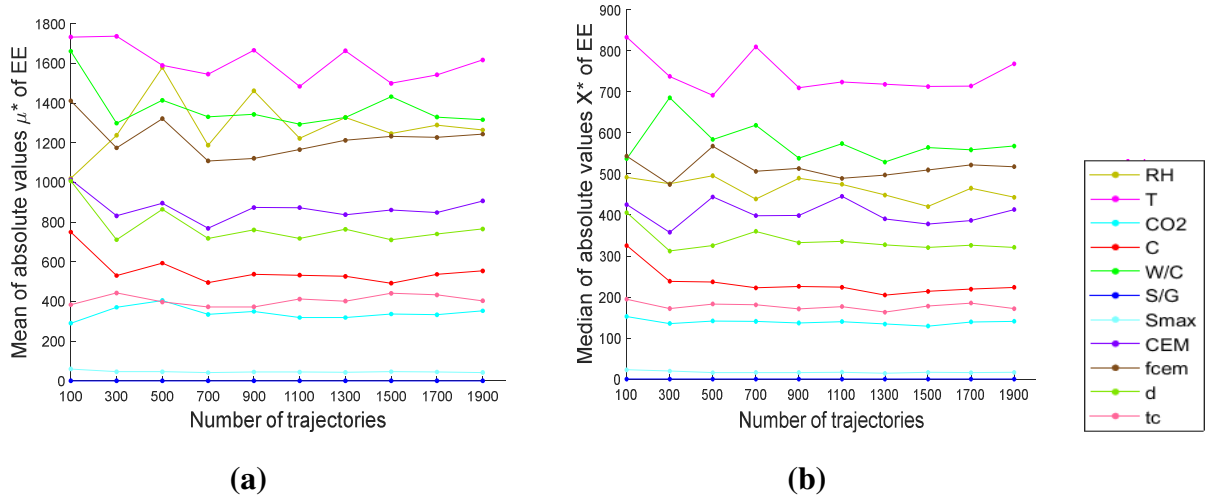
1123

|                                   | 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 |

1124 **Table S11** : The calculation cost according to the number of trajectories used in the application  
 1125 of Morris method to the carbonation model.

1126

1127

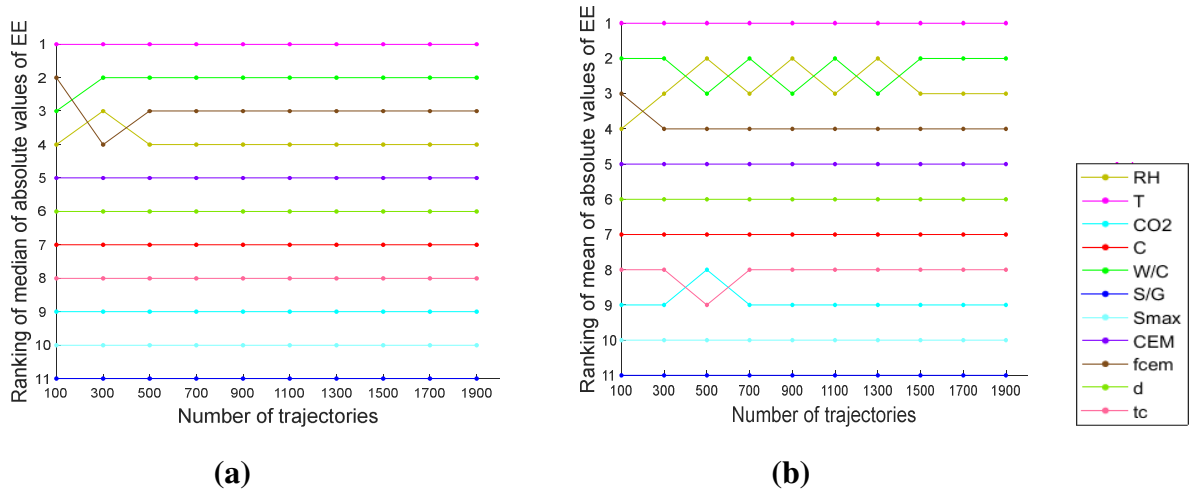


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1129

1130 **Figure S19** : Variations of the mean **(a)** and median **(b)** of absolute values of elementary effects  
 1131 (EE) for input parameters of the carbonation model by applying the Morris method.

1132



1133

1134

1135 **Figure S20** : Ranking of input parameters of the carbonation model, when using mean **(a)** and  
 1136 median **(b)** of absolute values of elementary effects (EE) for the Morris method.