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# Sensitivity analysis of the parameters of a time-dependent alkali-silica reaction model

Guy-de-patience Ftatsi Mbetmi<sup>a,b,1</sup>, Stéphane Multon<sup>a</sup>, Thomas de Larrard<sup>a</sup>,  
Frédéric Duprat<sup>a</sup>, Daniel Tieudjo<sup>c</sup>

(a) *LMDC, Université de Toulouse, INSA, UPS, 135 Avenue de Rangueil, 31077 Toulouse cedex 04 France*

(b) **Laboratoire d'Analyses Simulations et Essais (LASE), Université de Ngaoundéré, IUT, P.O. Box 455, Ngaoundere, Cameroon**

(c) **Laboratoire de Mathématiques Expérimentales (LAMEX), Université de Ngaoundéré, ENSAI, P.O. Box 455, Ngaoundere, Cameroon**

**Abstract:** Alkali-silica reaction (ASR) expansion is due to a combination of chemo-mechanical mechanisms. To obtain realistic predictions, modelling developed at the material scale has to consider reactive transport and mechanical issues. Numerous input variables concerning aggregate and cement paste properties are thus necessary. The uncertainties that affect such variables make the prediction of the ASR phenomenon random and thus need to be considered in a probabilistic context. To reduce the stochastic dimension for a further probabilistic analysis, a sensitivity analysis using the Morris method is conducted here, at different dates, on an ASR model developed at the material scale. It is illustrated by a combined sensitivity analysis of both the total volume of ASR products formed over time and the corresponding expansion. The work shows the relative impact of transport and reactive mechanisms on ASR kinetics. Moreover, the most significant parameters are not the same for laboratory accelerated expansion tests as for real structures under low temperatures. This highlights the relative impact of ASR mechanisms according to temperature.

**Keywords:** Alkali-silica reaction (ASR), Sensitivity analysis, Monte Carlo simulation, Morris method, Reliability.

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<sup>1</sup> [guy.ftatsi@univ-ndere.cm](mailto:guy.ftatsi@univ-ndere.cm)

28

29 **Highlights:**

30 - A sensitivity analysis of alkali-silica reaction model parameters is performed,

31 - A method to compute multiple outputs sensitivity analysis is proposed,

32 - The method relies on using a cumulative frequency threshold value,

33 - ASR kinetics can be more sensitive to reactive mechanisms than to transport in old concrete,

34 - Environmental conditions impact the ranking of significant variables.

35

36 **List of abbreviations and symbols**

37

38 **Agg.:** Aggregates

39 **ASR:** Alkali-Silica Reaction

40  $(\mathbf{B}_{(k+1) \times k})$ : Lower triangular matrix

41 ***cdfreq***: cumulative decreasing frequency

42 **CNA0** ( $\mathbf{C}_{Na}^{cp}$ ): Initial concentration of alkali in cement paste

43 **COLC** ( $t_c$ ): Reaction rim thickness

44 **CONGRA** ( $\mathbf{C}_{agg}$ ): Volumetric concentration of aggregate per m<sup>3</sup> of concrete

45 **D:** Diameter

46  $(\mathbf{D}_{k \times k}^*)$ : Diagonal matrix whose diagonal terms randomly take the values 1 or -1

47 **DIFFG** ( $\mathbf{D}$ ): Alkali diffusion coefficients

48 **EE:** Elementary Effect

49  $(\epsilon_V(t))$ : REV ASR expansion over time

50 **(*f* or *Fixna*)**: Coefficient of alkali fixation - taken as the same for all classes

51 **FRAGRA(i)**: Fraction of the class *i* granular material in aggregates

52  $(\mathbf{J}_{(k+1) \times k})$ : Matrix of  $(k + 1)$  lines and *k* columns of ones

53 **(*k*)**: Number of input variables

54 **Max:** Maximum

55 **Min:** Minimum

56  $(\mu_i)$ : Means on *r* of the  $EE_i$

57  $(\mu_i^*)$ : Absolute means on *r* of the  $EE_i$

58 **(*p*)**: Number of levels of each variation range (with  $p > k$ )

- 59  $(\phi_{ai})$ : Fraction of aggregate of class  $i$
- 60  $(P_{k \times k}^*)$ : Matrix where each column and each line contain only one element equal to 1 and all the  
61 others are equal to 0
- 62 **POROG** ( $P_{agg}$ ): Porosity of aggregates
- 63 **POROMO**: Porosity of the cement paste
- 64  $(r)$ : Number of trajectories
- 65  $(R)$ : The ideal gas constant
- 66  $(R_{ai})$ : Radius of aggregate of class  $i$
- 67 **REV**: Relative Elementary Volume
- 68 **RH**: Relative Humidity
- 69 **RNS**: Number of mol of Na reacting with 1 mol of Si to form 1 mol of gel
- 70  $(S_i^*)$ : Global sensitivity indices of each variable
- 71  $(\sigma_i)$ : Standard deviation on  $r$  of the  $EE_i$
- 72 **SILSOL**: Amount of soluble silica
- 73  $(S_{thv})$ : Sensitivity threshold value
- 74  $(T)$ : Temperature
- 75  $(T_0)$ : Reference temperature of the LPC N° 44 test (311 °K)
- 76  $(V_{g(t)})$ : Total volume of gel formed over time
- 77 **VMGEL** ( $V_{gel}^{mol}$ ): Molar volume of ASR-created gel
- 78  $(Vn[L])$ : Levels vector
- 79  $(V_{por})$ : Rim volume surrounding reactive particles
- 80  $(X_{max}^i)$ : Maximum values of variables  $X_i$  with  $i = 1, \dots, k$
- 81  $(X_{min}^i)$ : Minimum values of variables  $X_i$  with  $i = 1, \dots, k$

## 82 **1. Introduction**

83 Alkali-aggregate reaction causes significant deleterious degradation in many concrete structures,  
84 especially those where the concrete saturation degree is permanently high, such as dams. The  
85 alkali-aggregate reaction studied here is the alkali-silica reaction (ASR). It takes place between the  
86 poorly crystallized siliceous phases of silica aggregates and the alkaline interstitial solution of  
87 concrete. This reaction results in the formation of a gel and / or crystallized products, which can  
88 pressurize the surrounding concrete, causing cracking and expansion. Modelling ASR at the  
89 material level involves the transport of ionic species in the aggregate, the reactive mechanisms of  
90 dissolution and precipitation, and the conservation of ionic masses. During the reactive processes,  
91 silanol and siloxane interact to create siliceous gels [1–3]. ASR models must take both chemical  
92 and physical aspects into account to obtain relevant predictions of the mechanical responses of  
93 affected structures.

94 Apart from the approximations associated with the accepted hypothesis, many uncertainties affect  
95 the variables of the model, make the prediction of the ASR phenomenon random, and require  
96 operations to be carried out in a probabilistic context. A recent study proposed by Saouma pointed  
97 out the importance of stochastic analysis for the evaluation of ASR-damaged dams [4]. A similar  
98 situation exists for the determination of the advancement of the reaction according to  
99 environmental conditions in order to obtain accurate assessment of the evolution of damage with  
100 time. For the purpose of probabilistic analysis of the functional reliability of dams, a methodology  
101 based on the use of surrogate models has been planned for further study. The model adopted in the  
102 present work is the one developed at the material scale in LMDC by Multon et al. [5]. It has been  
103 compared with experimental evidence in [6]. To reduce the large number of variables to be  
104 considered as random in a probabilistic context, a one-at-a-time sensitivity analysis is undertaken.  
105 The final number of variables resulting from the reduction process is called the effective  
106 dimension, a concept introduced by Paskov and Traub [7] in finance, then by Caflisch et al. [8] in  
107 engineering. Later on, Kucherenko et al. [9] proposed the use of global sensitivity analysis with  
108 Sobol indices to obtain a model effective dimension. Riahi [10] developed an approach that  
109 consists of calculating the stochastic effective dimension with the Morris method. The present  
110 work extends that approach to multiple outputs and time dependent sensitivity analysis. The  
111 Morris method is used here to reduce the stochastic dimension, and so the computational cost, of  
112 our model rather than enhancing its predictive capabilities as in [11]. Additionally, we combine  
113 the sensitivity analyses performed at different dates to consider the time-dependency of the model  
114 in the present study.

115 Before the description of the ASR model used in this paper, a review of ASR modelling is  
116 proposed, followed by a presentation of the variation range of each input variable obtained with  
117 some Monte Carlo simulations to fit the experimental results of the ASR accelerated test LPC N°  
118 44 [12–15], carried out on cores drilled from Song Loulou dam in Cameroon [16] thirty years after  
119 its commissioning. Then, the Morris method is presented and an algorithm proposed to select  
120 variables on the basis of a combined sensitivity analysis. Finally, the sensitivity study is carried  
121 out on the selected model outputs. The most important variables are identified for each of the  
122 outputs, and from the combined sensitivity analysis, for different environmental conditions.

## 123 **2. Modelling Alkali-Silica Reaction at material scale**

### 124 **2.1. Literature review**

125 Alkali-Silica Reaction is caused by the chemical attack of specific silica aggregates and results in  
126 expansion and cracking of concrete. ASR modelling is thus an ambiguous term as the different  
127 models found in the literature can be centred on different aspects of physics. Some numerical  
128 works focus on mechanical considerations [17–25], some others analyse only the chemical  
129 advancement [26–31], while a third type of works consider the combination of physico-chemical  
130 mechanisms with mechanical considerations [5, 32–38]. To be realistic, ASR modelling should  
131 take into account:

- 132 - Transport for ions, water and ASR gels [5,26,28–30,32–38]: Before attacking aggregate,  
133 hydroxyl ions have to come into contact with amorphous silica (diffusion of ions in cement  
134 paste and aggregate). The ion diffusion is only possible if the porosity is sufficiently  
135 saturated in water and, to form, ASR gels absorb water (effect of water diffusion and  
136 permeability in concrete). Once formed, ASR gels under pressure just after their formation  
137 can partially move into the concrete porosity and induce cracking (ASR gel permeation).
- 138 - Thermodynamics [27,28,31]: ASR is the result of the aggregate dissolution (reaction  
139 between hydroxyl ions and amorphous silica) and of the precipitation of gels (reaction  
140 between silicic acid and alkali). These chemical reactions can be modelled by  
141 thermodynamic equilibrium [27,28] or by kinetics laws [5,39,40].
- 142 - Mechanics [5,17,18,20–25,32,41–43]: The formation of ASR gels in hardened concrete  
143 leads to cracking and expansion. Fracture or damage mechanics is necessary to evaluate  
144 the mechanical properties after degradation. Concrete creep has to be taken into account as  
145 it impacts the development of cracking.

146 In the literature, ionic or water transports are often considered as the processes controlling ASR  
147 kinetics. Recent works [28,39] have shown the importance of considering both transport and the

148 kinetics of chemical reactions to obtain realistic representations of rapid and slow reactive  
149 aggregate, e.g. the attack pattern observed in the literature [44]. Therefore, ASR modelling at  
150 material scale should be performed in a reactive transport framework. This leads to modelling with  
151 numerous input data. These data are affected by uncertainties and the prediction of ASR by such  
152 modelling is thus a random phenomenon. A probabilistic context can help to obtain reliable  
153 predictions. Among the few models eligible for the new approach that we intend to develop,  
154 namely the recalculation of ASR-affected structures from a microscopic model based mainly on  
155 measurable physical parameters, we chose the ASR model presented in [5] as it combines  
156 transport and reactive mechanisms.

157

## 158 **2.2. Physico-chemical ASR modelling**

### 159 *2.2.1 General modelling*

160

161 The ASR model used in this work considers the definition of a representative elementary volume  
162 (REV) of concrete that contains both cement paste and aggregate particles, reactive or not, of  
163 different sizes (Fig. 1). The REV is the smallest volume that represents the behaviour of the real  
164 concrete volume. Geometrical parameters thus have a large place in this modelling to characterize  
165 the size of reactive aggregates (minimal diameter of an aggregate class, DMIN and maximal  
166 diameter, DMAX) and the aggregate distribution (volumetric aggregate concentration –  
167 CONGRA, and fractions of each aggregate size – FRAGRA) presented in Table 1. Three granular  
168 classes are considered and the number (a) in Table 1 is associated with the aggregate class ( $a =$   
169 1,2,3).

170 The model developed at LMDC is based on the following chemical mechanisms:

171 - the diffusion of alkali into the aggregate particles (Fig. 1). Only one transport mechanism is  
172 considered. It is sufficient to reproduce a large number of experimental tests in saturated  
173 conditions [5,6,39]. For this part, the parameters of the model are the initial alkali  
174 concentration (CNA0), the aggregate porosity (POROG) and the coefficient of diffusion of  
175 alkali in aggregate (DIFFG) in Table 1.

176 - production of ASR gel (Fig. 1) and decrease of the alkali concentration in the cement paste  
177 relatively to their consumption by the new products to represent the reactive mechanisms.  
178 The maximal number of moles produced by ASR depends on the initial content of reactive  
179 components (the alkali concentration – CNA0 and the reactive silica content in aggregate –  
180 SILSOL) and on the ratio  $\text{Na}_2\text{O}_{\text{eq}}/\text{SiO}_2$  in the gel (RNS in Table 1). The gel volume is

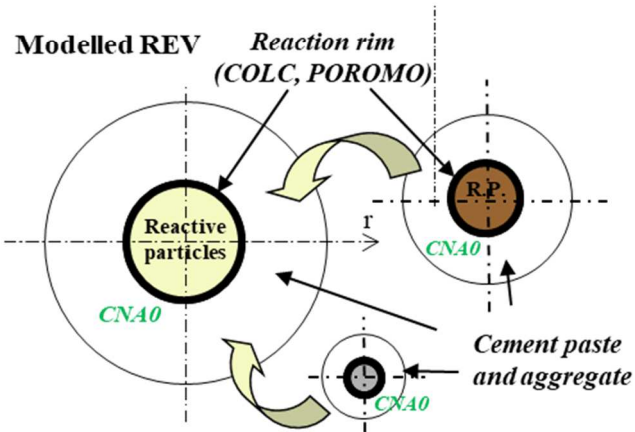
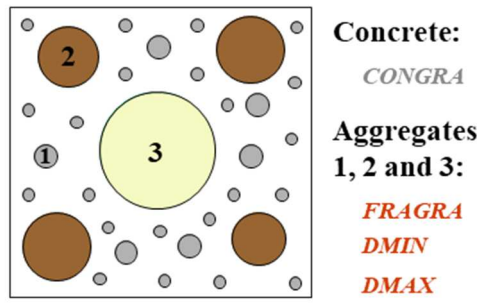


181 proportional to the number of gel moles and to the molar volume of ASR gels (VMGEL).  
182 The kinetics of gel production is driven by the coefficient of alkali fixation (FIXNA), which  
183 quantifies the fixation of alkali by the gel and thus the creation of gel.

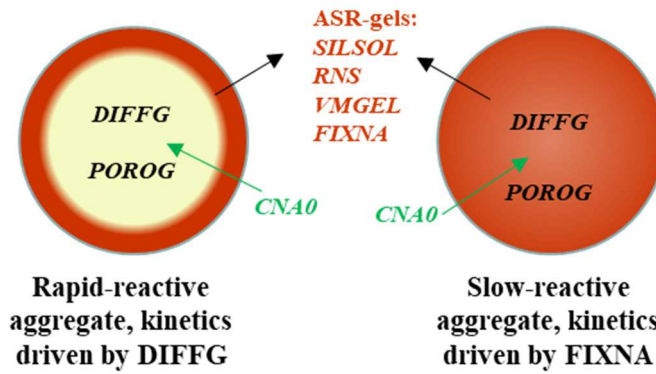
184 - permeation of gels around reactive sites in aggregate and paste porosity [32] and formation  
185 of rims around reactive aggregate [45]. For the sake of simplicity, the volume of gels filling  
186 pores and the volume of gels necessary to form the rims are modelled by an equivalent  
187 thickness (COLC) between cement paste and aggregate (Fig. 1). In reality, this volume of  
188 gel is accommodated in all the pores available in the aggregate and surrounding cement  
189 paste. In the rim, the porosity of the cement paste (POROMO) is assumed to be partly filled  
190 by gels. The gel produced once the rim is formed exerts significant pressure on the  
191 surrounding aggregate and cement paste and causes the REV expansion and cracking.

192

**Representative Elementary Volume**



**Modelled aggregate**



193

194 **Fig. 1.** Definition of the Relative Elementary Volume [5] and model parameters

195

196

197

198

**Table 1.** Ranges of variations of the input variables of the model

Concrete Parameters					
Description	Abbreviation	Symbol [5]	Initial Range	Final Range	Unit
Minimum diameter of the smallest granular class	DMIN(1)	$R_{(a=1,2,3)} = (DMIN(a) + DMAX(a)) / 2$	0 to 2	0 to 2	mm
Minimum diameter of the intermediate granular class	DMIN(2) = DMAX (1)		4 to 6	4 to 6	mm
Minimum diameter of the largest granular class	DMIN(3) = DMAX (2)		10 to 20	10 to 20	mm
Maximum diameter of the largest granular class	DMAX(3)		32 to 125	32 to 125	mm
Volumetric concentration of aggregate per m <sup>3</sup> of concrete	CONGRA	$C_{agg}$	0.6 to 0.75	0.6 to 0.75	-
Fraction of the smallest granular class in aggregates	FRAGRA(1)	$\phi_{(a=1,2,3)} = \text{Function of } (FRAGRA(a), SILSOL(a))$	0.25 to 0.55	0.25 to 0.55	-
Fraction of the medium and large granular class in aggregates	FRAGRA(2) = FRAGRA(3)		0.05 to 0.25	0.05 to 0.25	-
Physicochemical Parameters					
Description	Abbreviation	Symbol [5]	Initial Range	Final Range	Unit
Initial concentration of alkali in cement paste	CNA0	$C_{Na}^{cp}$	100 to 800	100 to 250	mol/m <sup>3</sup>
Amount of soluble silica for the smallest granular class (Sand)	SILSOL(1)	$\phi_{(a=1,2,3)} = \text{Function of } (FRAGRA(a), SILSOL(a))$	1000 to 5000	1000 to 3000	mol/m <sup>3</sup> of aggr.
Amount of soluble silica taken for the other granular classes and average reactivity	SILSOL(2) = SILSOL(3)		1000 to 5000	1000 to 3000	mol/m <sup>3</sup> of aggr.
Porosity of the cement paste	POROMO	$P_{cp}$	0.1 to 0.3	0.1 to 0.3	-
Porosity of small aggregates	POROG(1)	$P_{agg1}$	0.01 to 0.05	0.01 to 0.05	-
Porosity of aggregates taken for the other granular classes	POROG(2) = POROG(3)	$P_{agg2,3}$	0.01 to 0.05	0.01 to 0.05	-
Reaction rim thickness for small aggregates	COLC(1)	$t_{c(a=1)}$	1 to 15	1 to 10	μm
Reaction rim thickness for other aggregates	COLC(2) = COLC(3)	$t_{c(a=2,3)}$	1 to 15	1 to 10	μm
Alkali diffusion coefficients for small aggregates	DIFFG(1)	$D_{(a=1)}$	2.10 <sup>-13</sup> to 7.10 <sup>-13</sup>	2.10 <sup>-13</sup> to 7.10 <sup>-13</sup>	m <sup>2</sup> /s
Alkali diffusion coefficients for other aggregates	DIFFG(2) = DIFFG(3)	$D_{(a=2,3)}$	2.10 <sup>-13</sup> to 7.10 <sup>-13</sup>	2.10 <sup>-13</sup> to 7.10 <sup>-13</sup>	m <sup>2</sup> /s
ASR gel parameters					
Description	Abbreviation	Symbol [5]	Initial Range	Final Range	Unit
Molar volume of ASR-created gel	VMGEL	$V_{gel}^{mol}$	1.10 <sup>-5</sup> to 10.10 <sup>-5</sup>	1.10 <sup>-5</sup> to 1.6.10 <sup>-5</sup>	m <sup>3</sup> /mol
Number of mol of Na reacting with 1 mol of Si to form 1 mol of gel	RNS	$Ratio Na_2O/SiO_2$	0.2 to 0.8	0.39 to 0.59	-
Coefficient of alkali fixation taken as the same for all classes	FIXNA	$f$	-1.10 <sup>-7</sup> to -1.10 <sup>-9</sup>	-1.10 <sup>-7</sup> to -1.10 <sup>-9</sup>	m <sup>3</sup> /m <sup>3</sup> /s

200

201 The constitutive equations of the ASR gel expansion model have been presented and explained in  
 202 [5]. Both rapid and slow reactive aggregates can be modelled (Fig. 1) through the combination of

203 diffusion and reactive mechanisms [39]. Only one point has been modified from the initial version  
 204 of the model [5]: the existence of a constant threshold alkali concentration above which ASR can  
 205 occur is questionable [39,46]. This threshold is probably dependent on chemical conditions, e.g.  
 206 calcium concentration [39]. In the present work, no alkali concentration threshold is assumed. All  
 207 the alkali ions can participate in gel formation.

208 The input variables analysed in this paper are all summarized in Fig. 1 and Table 1. The ranges  
 209 were derived from our expertise combined with the information available in the literature, as  
 210 explained in the next section. It can be deemed that they contain about 95% of the consistent  
 211 knowledge of the parameters in question, as justified in part 2.3.

212

### 213 2.2.2 Consideration of environmental conditions

214 In the model, the temperature impacts both the transport, through the alkali diffusion coefficient in  
 215 the aggregate, and the reactive mechanisms (dissolution of silica and ASR-gel formations),  
 216 through the single simplified equation of alkali fixation [39]. As shown by the literature, reactive  
 217 mechanisms are usually more sensitive to temperature than diffusive transport [27,47,48]. This is  
 218 taken into account through the activation energy of each phenomenon,  $E_A^{Fixna} = 78$  kJ/mol for the  
 219 alkali fixation (Eq. 1), versus  $E_A^{DiffG} = 20$  kJ/mol for the alkali diffusion (Eq. 2).

$$220 \quad Fixna(T) = Fixna_0 e^{\frac{E_A^{Fixna}}{R} \left( \frac{1}{T} - \frac{1}{T_0} \right)} \quad (Eq. 1)$$

$$221 \quad DiffG(T) = DiffG_0 e^{-\frac{E_A^{DiffG}}{R} \left( \frac{1}{T} - \frac{1}{T_0} \right)} \quad (Eq. 2)$$

222 where  $R = 8.31 J.K^{-1}.mol^{-1}$  the ideal gas constant;  $T$  (°K), temperature;  $T_0 = 311$  °K,  
 223 temperature of the expansion test performed on cores (LPC N° 44), test taken as a reference in this  
 224 work.

225 The variation of relative humidity can be considered in the modelling through the variation of the  
 226 diffusion coefficient with the saturation degree of the concrete [49]. The impact of the variation of  
 227 moisture on the model response has not been evaluated in the paper because the specimens during  
 228 the accelerated test (RH 95%) and the concrete of the Song Loulou dam (RH > 80%) [50] were at  
 229 very high and quasi-constant relative humidity during ASR expansion. Concerning the alkali  
 effect on expansion, alkali leaching can occur during the expansion test and can be considered by  
 the modelling [39]. However, the cores extracted from the concrete of the Song Loulou dam had a

230 diameter of 140 mm. Therefore, alkali leaching was neglected as Lindgård et al. showed that the  
231 loss of alkali was lower than 10% for specimens with sizes greater than 100 mm [51].

232  
233 **2.3. Independent input variables of the model and range of variation**

234 Following a study commissioned by the dam manager, core specimens were drilled from the Song  
235 Loulou hydropower dam (Fig. 2), to undergo various tests including the accelerated swelling test  
236 LPC N°44 and the petrographic study carried out by the former LCPC (Laboratoire Central des  
237 Ponts et Chaussées) in 2011. LPC N°44 is an expansion test on a core extracted in an ASR-  
238 affected concrete structure. The core had to be equipped with plots for strain measurement and  
239 kept in a 38 °C and 95% RH environment. The evolution of the length had to be noted regularly  
240 over 52 weeks [12]. In order to obtain homogeneous conditions, cores are usually stored in small  
241 containers (28 cm x 23 cm x 40 cm in height) [13].

242 The cores presented in Fig. 2 were extracted from the following points of the Song Loulou dam: at  
243 the base of buttress 45 (C45-1), on the top of spillway pile 12 (P12-1), on the right bank of the  
244 spillway pile (P12-2).



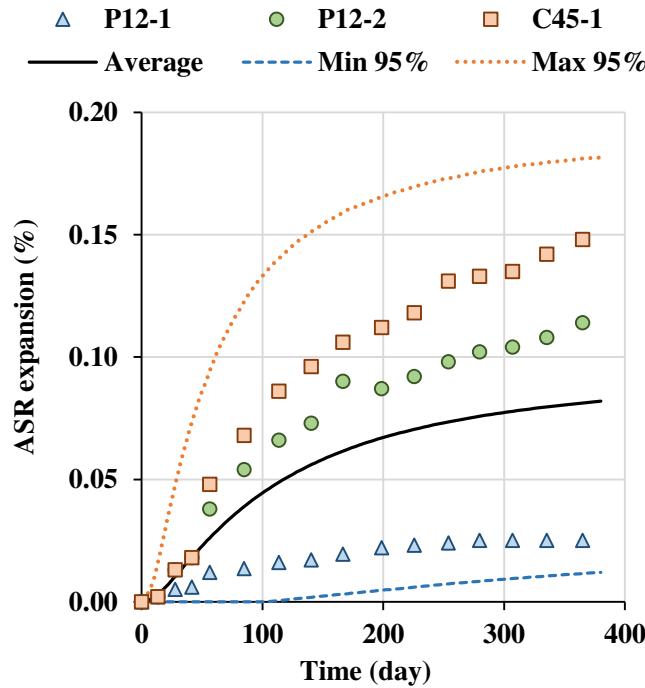
245  
246 **Fig. 2.** Cores extracted from Song Loulou dam for the LPC N° 44 test, credit to Guedon -  
247 IFSTTAR 2010

248 For our sensitivity analysis to be relevant using the proposed method, it is necessary to define the  
249 real ranges of the independent input variables. Twenty of them have been identified for the model,  
250 (**Table 1**), considering that the smallest granular class (sand) has different physicochemical  
251 properties from the middle and large classes (gravel and stones). This hypothesis is based on the  
252 dam construction data and the 2011 petrographic observations. Additionally, in the case of cores

253 drilled from the structures, aggregates had already been attacked in the structure, before the  
254 laboratory tests. Due to diffusive mechanisms, the chemical advancement in sand is potentially  
255 larger than the advancement in gravel and stones, inducing different physicochemical properties.

256 The initial ranges of the input variables were defined according to literature and Song Loulou dam  
257 construction reports. The first 7 variables in **Table 1** are physical variables whose ranges were  
258 deduced from the concrete formulation of the Song Loulou dam, and also in accordance with [52].  
259 The porosity range was measured on extracted cores. The initial ranges of the twelve other  
260 variables were defined from the literature [5,6,34,53]. In addition to these three references used for  
261 all the variables, we used specific references for some variables: values for the initial alkali  
262 concentration, “CNA0” and the molar volume of ASR gels, “VMGEL” were from [54] and, for  
263 the two coefficients of alkali diffusion in aggregate “DIFFG”, the values were from [47].

264 These ranges were then refined by using Monte Carlo simulations [55,56], in order to reflect the  
265 reality of our study case. For that purpose, on the basis of the results obtained from tests carried  
266 out on ten cores [16], three reference data were selected: P12-1 and P12-2 were drilled in Pier 12  
267 of the dam and represent the minimum and the average kinetics respectively (Fig. 3), C45-1 was  
268 drilled from the basis of Buttress 45 and represents the maximal ASR kinetics obtained for the  
269 expansion tests performed on the concrete dams. Some 2000 simulations to approach the final  
270 intervals were run by progressively reducing the initial intervals. Then 10 000 simulations were  
271 performed to confirm the ranges which best fit the experimental curves. It is important to note that  
272 the intervals of the variables deduced from Song Loulou construction expansion tests were kept  
273 constant during the process. The aim of the procedure is that the 95% confidence interval should  
274 frame the extreme experimental values (Fig. 3). The final ranges used in the sensitivity analysis  
275 below are shown in Table 1. The statistics computed from the Monte Carlo simulations show that  
276 the experimental values are well within the 95% confidence interval of results from the model  
277 (Fig. 3). The final ranges given in Table 1 can be useful to evaluate the potential expansion of  
278 concrete damaged by ASR with similar characteristics.



279

280 **Fig. 3.** Kinetics of minimal, average and maximal swelling for a quantile of 95% - 10 000  
 281 simulations - Final ranges (dots: experimental data, lines: model)

282 **3. Morris method and variable selection algorithm**

283 The Morris method [57–59] allows input variables to be classified according to their importance  
 284 with regard to their influence on the response of a model. It is based on the assumption that, by  
 285 varying variables of the same relative pitch one at a time, the one that causes the greatest variation,  
 286 expressed in statistical terms, on the output is the most important. The process results in the  
 287 stochastic dependence between variables not being taken into account. So, to use that method,  
 288 variables need to be independent.

289 **3.1. Trajectories and Elementary Effects (EE)**

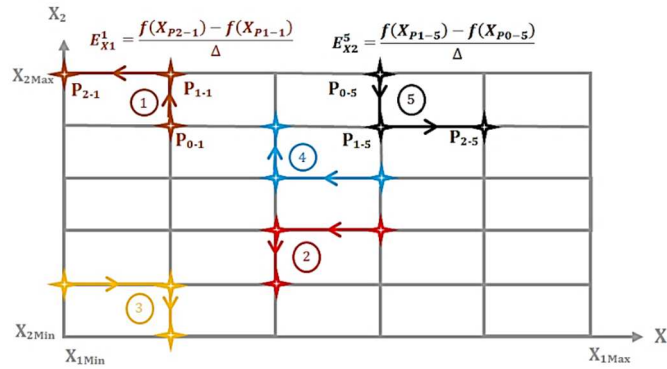
290 The first step is to construct trajectories that will be used to calculate the elementary effects and  
 291 the Morris sensitivity analysis indicators. For that purpose, we divide the variation range of each  
 292 of the  $k$  input variables into  $p$  levels ( $p > k$ ) from the minimum to the maximum with a pitch (or  
 293 perturbation  $\Delta = 1 / (p - 1)$ ). Then, we build  $r$  trajectories each consisting of  $k + 1$  points and  
 294 their respective responses. The first point is drawn randomly and the other  $k$  points are calculated  
 295 so that just one of the  $k$  variables changes by  $\pm \Delta$  from one calculated point to another. Each  
 296 trajectory is used to determine an Elementary Effect (EE) of each variable according to the  
 297 expression (Eq. 3)

$$EE_i = f(X_1, \dots, X_i + \Delta, \dots, X_k) - f(X_1, \dots, X_i, \dots, X_k) / \Delta \quad (\text{Eq. 3})$$

298

299 The computation of the Morris indicators requires several elementary effects per variable and  
 300 therefore the computation of several trajectories. Fig. 4 shows five trajectories for two variables  
 301 ( $r = 5, k = 2$ ), with the expressions of some of the resulting elementary effects. The first point  
 302 of each of these trajectories is drawn randomly and the other two points ( $k + 1 = 3$  points per  
 303 trajectory) are computed in order to have only one relative variation of  $\pm \Delta$  between two  
 304 consecutive points.

305 Generally, a trajectory can be constructed by matrix computation according to equations (Eq.4)  
 306 and (Eq.5), the details of which are given in [59]. However, a clear description of the constitutive  
 307 elements of these equations is given in the algorithm in **Appendix A**.



308

**Fig. 4.** Example of elementary effects for  $k = 2, r = 5, p = 6$  ( $\Delta = 0.2$ )

309

310

$$B_{(k+1) \times k}^* = J_{(k+1) \times 1} \cdot X_{1 \times k}^* + \left(\frac{\Delta}{2}\right) \cdot \left[ (2B_{(k+1) \times k} - J_{(k+1) \times k}) \cdot D_{k \times k}^* + J_{(k+1) \times k} \right] \cdot P_{k \times k}^* \quad (\text{Eq.4})$$

311 The points of the trajectory are given by:

312

$$X_{i=1,2,\dots,k+1;j=1,2,\dots,k}^{i,j} = X_{min}^j + B_{i,j}^* (X_{max}^j - X_{min}^j) \quad (\text{Eq.5})$$

313

### 3.2. Sensitivity analysis indicators and selection of variables

314 Sensitivity analysis indicators are computed from elementary effects statistics, equation (Eq.6)  
 315 from [58], and equation (Eq.7) deduced from [60].  $\mu_i$  and  $\sigma_i$  are respectively the mean value and  
 316 standard deviation of the elementary effects.  $\mu_i^*$  is the mean value of the absolute elementary  
 317 effects. High values of  $\mu_i^*$  reveal a strong sensitivity to the variables considered and  $\sigma_i$  is related to  
 318 non-linear aspects.  $S_i^*$  is an indicator of global sensitivity. The number of trajectories required is  
 319



320 that from which these indicators become constant. The larger that number is, the more accurate are  
 321 the results, but the calculation cost also increases.

$$\mu_i = \sum_{j=1}^r EE_{i,j}/r, \mu_i^* = \sum_{j=1}^r |EE_{i,j}|/r, \sigma_i = \sqrt{\frac{1}{(r-1)} \times \sum_{j=1}^r (EE_{i,j} - \mu_i)^2} \quad (\text{Eq.6})$$

$$S_i^* = (\mu_i^{*2} + \sigma_i^2) / \sum_{i=1}^n (\mu_i^{*2} + \sigma_i^2) \quad (\text{Eq.7})$$

322

### 323 3.3. Variables selection algorithm

324 The selection process used in the present study is summarized in the Algorithm in Appendix A.  
 325 For a single output, the variables for which the cumulative decreasing global sensitivity indices are  
 326 lower than a threshold value will be selected. For multiple outputs, we sum the global sensitivity  
 327 indices of each variable on all outputs and compute the cumulative decreasing frequency of each  
 328 sum. Then the variables with a cumulative decreasing frequency less than a threshold value are  
 329 selected. Commonly, the threshold values used in sensitivity analysis are either 90%, for a narrow  
 330 selection window, or 99%, for a large selection window. In the applications given in the following  
 331 parts, a medium sized selection window with a threshold value of 95% is chosen.

### 332 4. Sensitivity analysis of the ASR model during accelerated expansion test

333 The ASR model developed in the LMDC [5] can be used to evaluate the production of gel during  
 334 LPC accelerated test N° 44 on a test specimen. Tests are carried out at 38 °C and 100% relative  
 335 humidity. Using the Morris method with the parameters  $k = 20, r = 600, p = 81$  ( $\Delta = 0.0125$ ),  
 336 the respective variation ranges for the input variables on various outputs of interest deduced from  
 337 the model (Table 1) are considered. Values of r and p lead to an accurate sensitivity analysis. Let  
 338 us recall that we used three granular classes when implementing the model, where digits 1, 2 and 3  
 339 are associated with small, medium and large sizes respectively. The sensitivity of the model is first  
 340 analysed according to the two main outputs:

341 - the total volume of gel formed during time  $t$ :

$$V_g(t) = \sum_{i=1}^3 V_{gi}(t) \quad (\text{Eq.8})$$

342 - and the corresponding ASR expansion evaluated in this work by the following equation:

$$\varepsilon_V(t) = \sum_{i=1}^3 \frac{V_{gi}(t) - V_{por\_i}}{V_{VERi}} \quad (\text{Eq.9})$$

343 with  $V_{por}$ , the rim volume surrounding reactive particles [5].

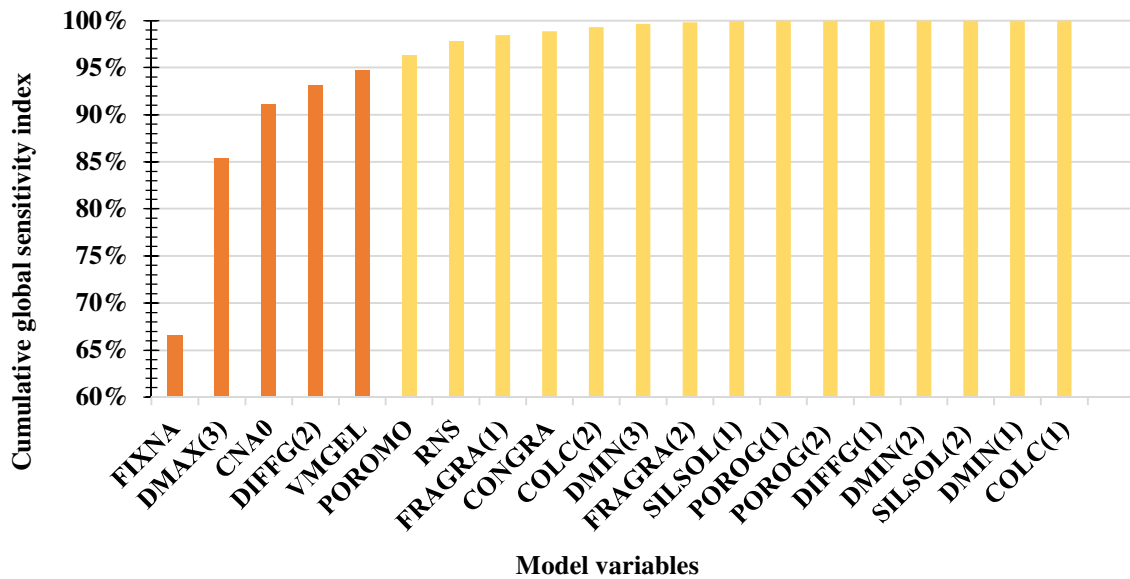
344 The first output is related to the chemical aspects of ASR, while the second output is the one that  
 345 effectively impacts the mechanical behaviour of the concrete.

346  
 347 **4.1. Sensitivity of the total volume of gel formed during time  $V_g(t)$**

348 *4.1.1 Sensitivity analysis at different dates*

349 The analysis of the sensitivity of the total volume of gel formed during time ( $V_g(t)$ ) was  
 350 performed for 4 different dates: 10, 100, 180, and 365 days after the beginning of the test, in order  
 351 to regularly cover the ASR accelerated test duration. Fig. 5 shows the results obtained at 365 days.  
 352 The five variables that can be considered important, since their cumulative decreasing global  
 353 sensitivity index is less than or equal to 95% ( $S_{thv} = 95\%$ ) are those represented by the dark bars  
 354 on the histogram of Fig. 5: the coefficient of alkali fixation (FIXNA), the size of the biggest  
 355 aggregate (D<sub>MAX</sub>(3)), the initial alkali concentration (C<sub>NA0</sub>), the coefficient of diffusion of the  
 356 biggest aggregate (D<sub>IFFG</sub>(2)=D<sub>IFFG</sub>(3)) and the molar volume of ASR gels (V<sub>MGEL</sub>). Fig. 6  
 357 shows the ranking of the important variables for each of the four dates.

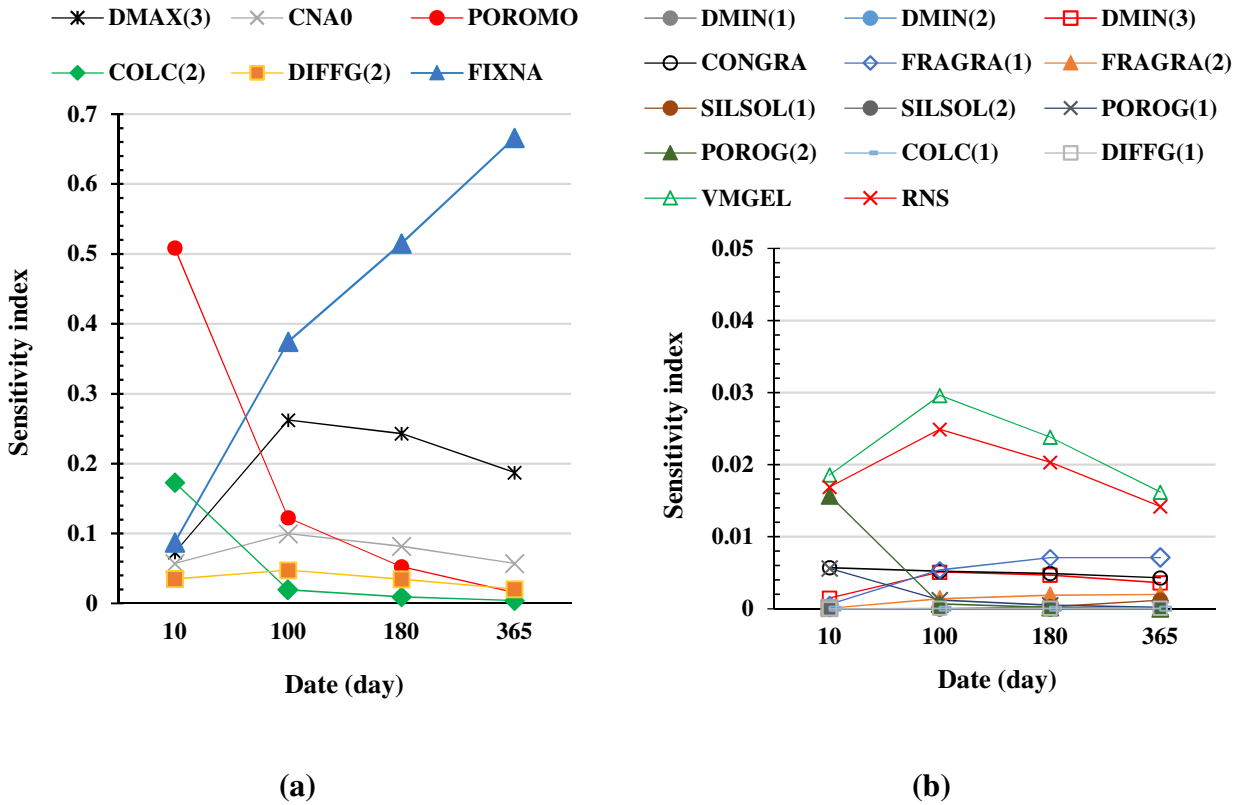
358



359  
 360 **Fig. 5. Global cumulative sensitivity index of  $V_g(t = 365 \text{ days})$**

361

362



363 **Fig. 6.** Global sensitivity index for  $V_g(t)$  at different times: parameters with high sensitivity (a)  
 364 and parameters with sensitivity lower than 0.04 for all times (b)

365 One remarkable fact is that both the thickness of the reactive rim for medium and large aggregates,  
 366 namely “COLC(2)”, and the porosity of the mortar “POROMO”, which appear to be important at  
 367 10 days (i.e. at the initialization of the reaction), become less important with time. This highlights  
 368 the importance of these two parameters in the latency time of expansion (at the beginning, ASR  
 369 gels can migrate in the porosity close to the reactive sites without inducing expansion).  
 370 Conversely, the size of the largest aggregate, “DMAX(3)”, is less important at the beginning of  
 371 expansion than later. At the beginning of expansion, alkali has not had time to reach the reactive  
 372 silica in the largest aggregates and they cannot produce gels.

373 The global sensitivity index of the alkali fixation coefficient “FIXNA” increases throughout the  
 374 period. This can be physically justified by the fact that the alkali diffusion phenomenon, which is  
 375 dominant in the beginning of the ASR reaction, gradually decreases, giving way to alkali fixation  
 376 by the gel. The two other important variables (“DIFFG(2)” and “CNA0”) have almost constant  
 377 sensitivity during the test period.

378

379

#### 380 4.1.2 Global indicator for sensitivity analysis for the whole period

381 As shown just above, the sensitivity of each parameter varies with time. It can be useful to  
382 combine the sensitivity at the different times in a single, global indicator. Thus, the parameter with  
383 the greatest impact during the whole period of expansion can be highlighted.

384 For each variable, the indicator is equal to the sum of the Morris global sensitivity at all dates  
385 investigated:

$$\sum_t S_i^{Vg(t)} = S_i^{Vg(10)} + S_i^{Vg(100)} + S_i^{Vg(180)} + S_i^{Vg(365)} \quad (\text{Eq.10})$$

386 The results are presented in Table 2. A corresponding frequency can be deduced by using the  
387 relative global sensitivity:

$$frq = 100 \frac{\sum_t S_i^{Vg(t)}}{\sum_i (\sum_t S_i^{Vg(t)})} \quad (\text{Eq.11})$$

388 The variables are sorted in decreasing order compared to this last indicator. The fourth column of  
389 Table 2 indicates the cumulative frequency, *cdfrq*, leading to the selection of the most influential  
390 variable for the whole period of expansion. The most influential variables have a  $cdfrq \leq S_{thv} =$   
391 95%. They are highlighted in Fig. 7.

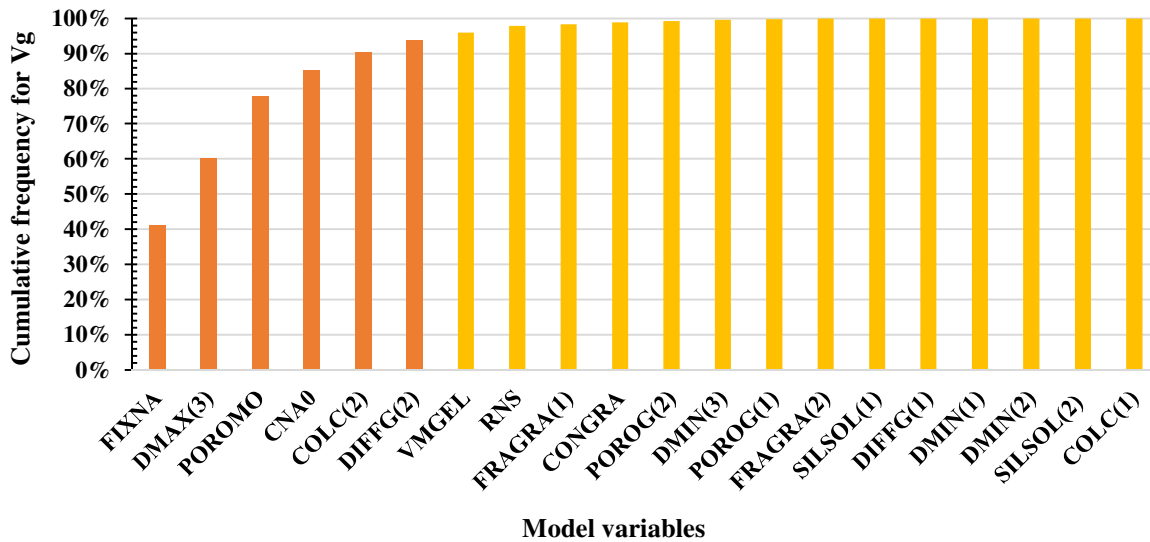
392

393

394 **Table 2.** Cumulative frequency on the sum of global sensitivity index of  $V_g$  for all dates

Description	$\sum_t s_i^{V_g(t)}$	frq (%)	cdfrq (%)	s.v.
<b>DMIN(1)</b>	0.000	0.000	<b>41.075</b>	<b>FIXNA</b>
<b>DMIN(2)</b>	0.000	0.000	<b>60.215</b>	<b>DMAX(3)</b>
<b>DMIN(3)</b>	0.015	0.373	<b>77.708</b>	<b>POROMO</b>
<b>DMAX(3)</b>	0.766	19.140	<b>85.115</b>	<b>CNA0</b>
<b>CONGRA</b>	0.020	0.503	<b>90.273</b>	<b>COLC(2)</b>
<b>FRAGRA(1)</b>	0.020	0.505	<b>93.725</b>	<b>DIFFG(2)</b>
<b>FRAGRA(2)</b>	0.005	0.135	95.930	VMGEL
<b>CNA0</b>	0.296	7.408	97.838	RNS
<b>SILSOL(1)</b>	0.002	0.038	98.343	FRAGRA(1)
<b>SILSOL(2)</b>	0.000	0.000	98.845	CONGRA
<b>POROMO</b>	0.700	17.493	99.260	POROG(2)
<b>POROG(1)</b>	0.007	0.187	99.633	DMIN(3)
<b>POROG(2)</b>	0.017	0.415	99.820	POROG(1)
<b>COLC(1)</b>	0.000	0.000	99.955	FRAGRA(2)
<b>COLC(2)</b>	0.206	5.158	99.993	SILSOL(1)
<b>DIFFG(1)</b>	0.000	0.007	100.000	DIFFG(1)
<b>DIFFG(2)</b>	0.138	3.453	100.000	DMIN(1)
<b>VMGEL</b>	0.088	2.205	100.000	DMIN(2)
<b>RNS</b>	0.076	1.908	100.000	SILSOL(2)
<b>FIXNA</b>	1.643	41.075	100.000	COLC(1)

395



396

397 **Fig. 7.** Cumulative frequency for  $V_g$  for the whole period

398

399 The most influential variables on ASR gel creation quantified by  $V_g$  would be: the coefficient of  
 400 alkali fixation “FIXNA”, the maximum diameter of the largest granular class “DMAX(3)”, the

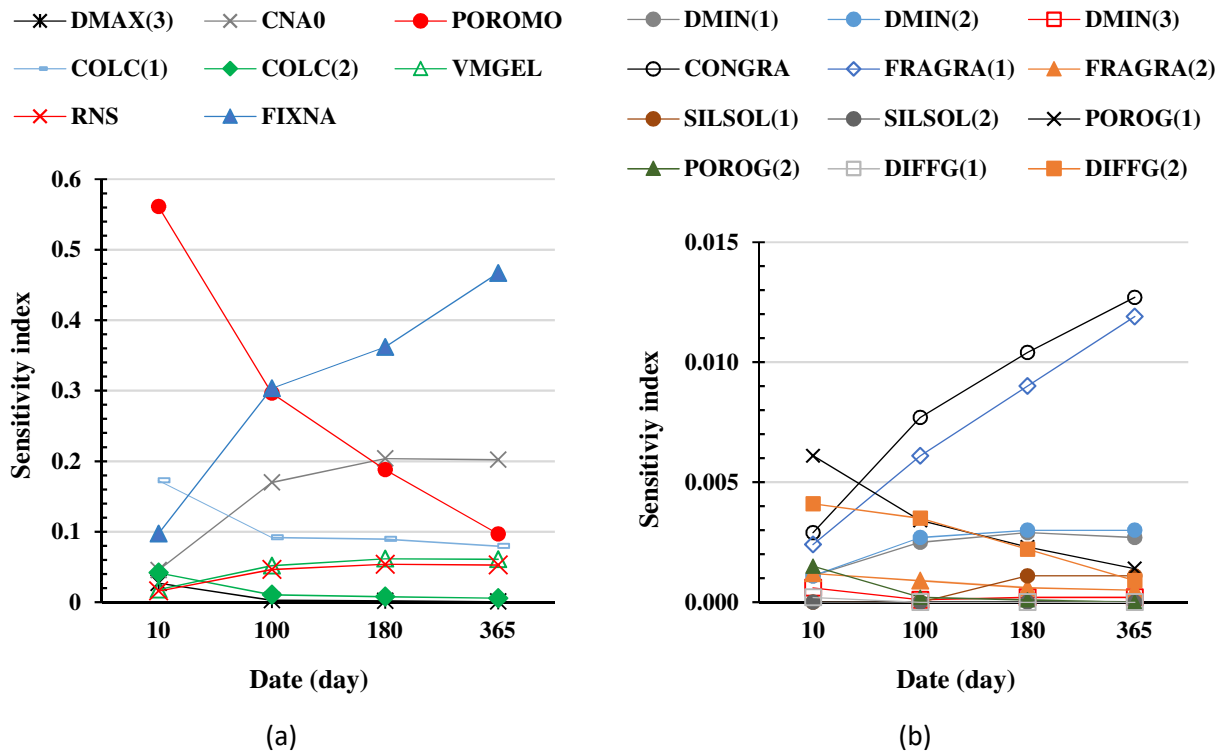
401 mortar porosity “POROMO”, the initial concentration of alkali in cement paste “CNA0”, the rim  
 402 thickness for medium and large sized aggregates “COLC(2)” and the coefficient of alkali diffusion  
 403 for medium and large sized aggregates “DIFFG(2)”.

404 **4.2. Results for the corresponding REV expansion during time  $\varepsilon_V(t)$**

405 *4.2.1 Sensitivity analysis at different dates*

406 The same procedure was used for the second output, namely the ASR expansion during time,  
 407  $\varepsilon_V(t)$ , for the same 4 dates as in the previous section. Fig. 8 summarizes the outcome of the  
 408 sensitivity analysis at the four chosen dates.

409



410

411 **Fig. 8.** Global sensitivity index of ASR expansion,  $\varepsilon_V(t)$ , at different times: parameters with the  
 412 highest sensitivity (a) and parameters with sensitivity lower than 0.015 for all times (b)

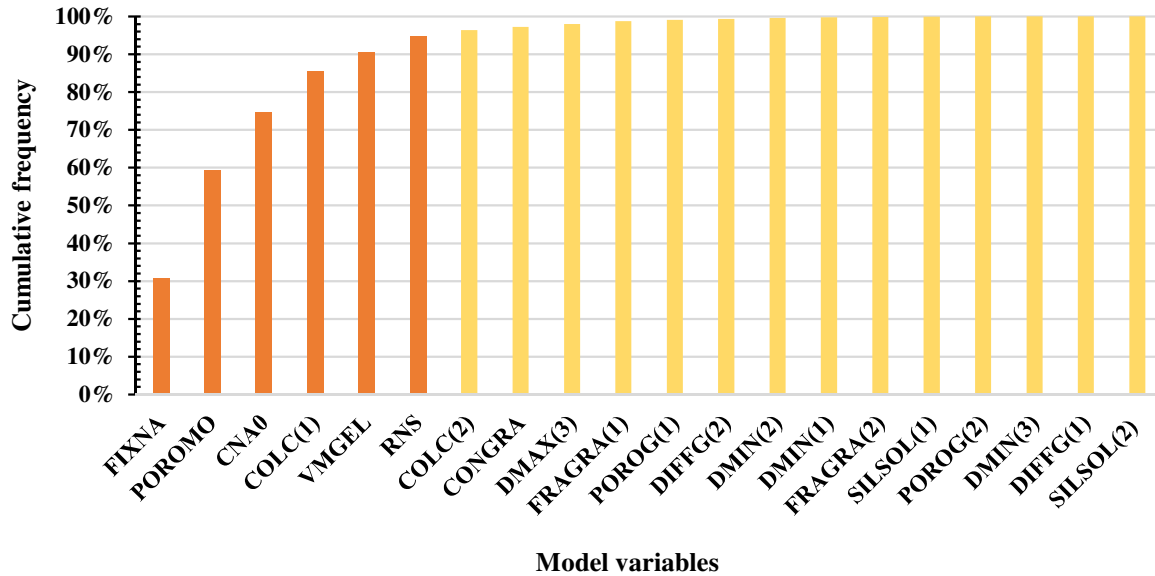
413 We can observe the same result concerning “POROMO” and “FIXNA” as in the previous  
 414 paragraph. Given that  $\varepsilon_V$  is REV relative data, the fact that small (respectively big) aggregates  
 415 have small (respectively big) REV volume as the divisor might explain why the maximum  
 416 diameter of the largest granular class DMAX(3), which appears to be important in the analysis of  
 417  $V_g(t)$ , disappears in the analysis of  $\varepsilon_V$ .

418

419

#### 420 4.2.2 Global indicator for sensitivity analysis

421 After using the same procedure as for  $V_g(t)$  with the data presented in Fig. 8, we obtained the  
422 overall result presented in Fig. 9 for the four dates.



423 **Fig. 9.** Cumulative frequency on the sum of global sensitivity index of ASR expansion for all  
424 dates

425 The six variables to be considered as having the most influence on the expansion quantified by  $\varepsilon_V$   
426 would be the coefficient of alkali fixation “FIXNA”, the mortar porosity “POROMO”, the initial  
427 concentration of alkali in cement paste “CNA0”, the rim thickness “COLC(1)”, the molar volume  
428 of ASR gel “VMGEL”, and the  $\text{Na}_2\text{O}_{\text{eq}}/\text{SiO}_2$  ratio “RNS”.

429

#### 430 4.3. Combined sensitivity analysis

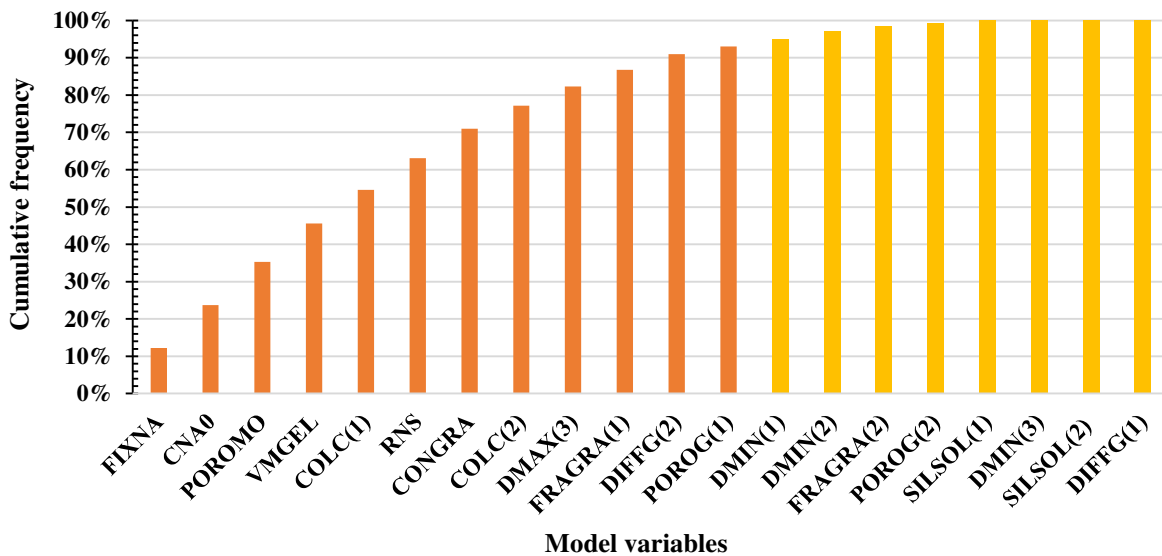
431 In the previous parts, the sensitivity of the model has been analysed for each output. In this part, a  
432 combined sensitivity analysis is proposed in order to point out the parameters with the greatest  
433 influence on several outputs of interest. To obtain complete and precise analysis, it is based on  
434 five outputs that can, at various times in the course of the phenomenon and at various levels,  
435 impair the functionality of the dam:

- 436 - the total volume of gel formed for five time-steps,
- 437 - the corresponding ASR expansions,
- 438 - the expansion rate at the same five time-steps,

- 439 - the advancement of ASR in terms of expansion (5, 25, 50, 75, 90, 95, 100% of the final
- 440 expansion),
- 441 - the time to reach the previous advancements.

442 In the following analysis, only cumulative frequency is presented. Using more outputs gives better  
 443 precision in the evaluation. The ranking of input parameters obtained is presented in Fig. 10.

444  
 445



446

447 **Fig. 10.** Cumulative frequency on the sum of global sensitivity index of all outputs

448 The increase of cumulative frequency with the number of parameters is more progressive than in  
 449 the previous analysis. This can be explained by the number of outputs taken into account here  
 450 which, in turn, increases the number of possibly influential parameters, reaching 60% of the  
 451 inputs.

452 The results confirm the prominence of the variable “FIXNA” compared to all the other variables  
 453 for expansion tests at 38 °C. The initial concentration of alkali in cement paste, “CNA0”, which  
 454 controls the attack range of aggregates, is the second most important parameter. This was not the  
 455 case in the two first analyses where this parameter was the fourth then the third most influential  
 456 parameter. All the other significant parameters of the two first analyses remain important in this  
 457 cumulative analysis and only their relative rank can be modified from one output to another.

458 Fig. 10 shows that most of parameters have some impact on the outputs of the model. This  
 459 analysis confirms the necessity to consider all the chemo-mechanical mechanisms quantified by  
 460 these parameters. Finally, the parameters with little impact are mainly: the reactive silica content



461 (because, in these calculations, the limiting species are the alkali ions), the diffusion coefficient in  
462 the sand (as the sand particles are small, the diffusion is always fast in these particles) and the  
463 smallest size of the reactive particles (DMIN(i)).

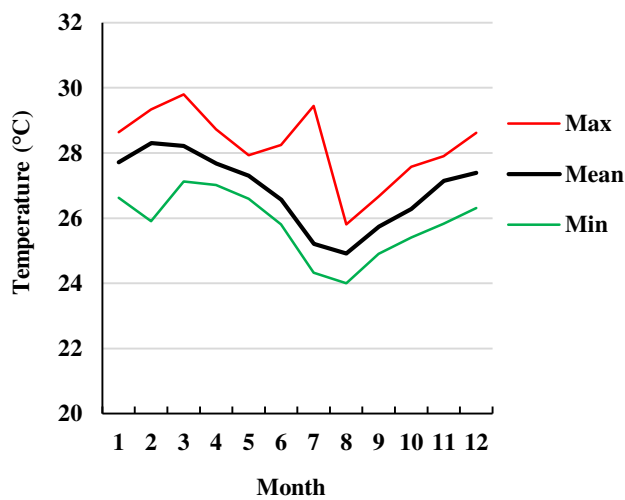
## 464 5. Sensitivity analysis for ASR under environmental conditions

### 465 5.1. Impact of temperature on the sensitivity of the model

466 Due to the very wet environmental conditions of the Song Loulou dam (external relative humidity  
467 usually above 80%) and to the presence of the water intake, the concrete of the dam is assumed to  
468 be saturated. The aim of this part is thus to analyse the impact of the temperature on the sensitivity  
469 of the model.

### 470 5.2. Impact of constant in-field temperature on the sensitivity

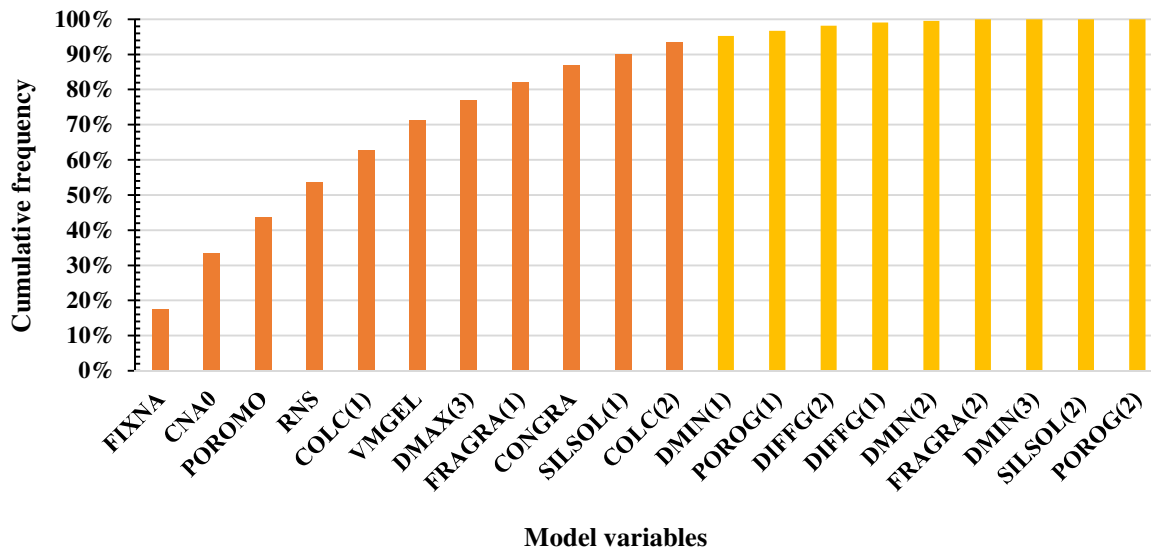
471 The impact of the temperature on the sensitivity of the model is first analysed on expansions  
472 evaluated for a constant temperature of about 29 °C, which corresponds to the highest mean  
473 temperature recorded close to Song Loulou dam from 1975 to 2008 (Fig. 11). This temperature is  
474 lower than the temperature of the expansion test (38 °C) and can thus affect the importance of  
475 each parameter of the model. The cumulative frequency obtained for all the outputs is presented in  
476 Fig. 12.



477

478 **Fig. 11.** Monthly mean temperature close to Song Loulou dam

479 The effect of a decrease of about 10 °C in the temperature is small (Fig. 12). The three most  
480 important parameters are the same (the alkali fixation, the initial alkali concentration and the  
481 mortar porosity). It is worth noting that the composition of ASR gels (through RNS, the Na<sub>2</sub>O /  
482 SiO<sub>2</sub> ratio) is more important at 29 °C than at 38 °C (it gains two places in the ranking).



483

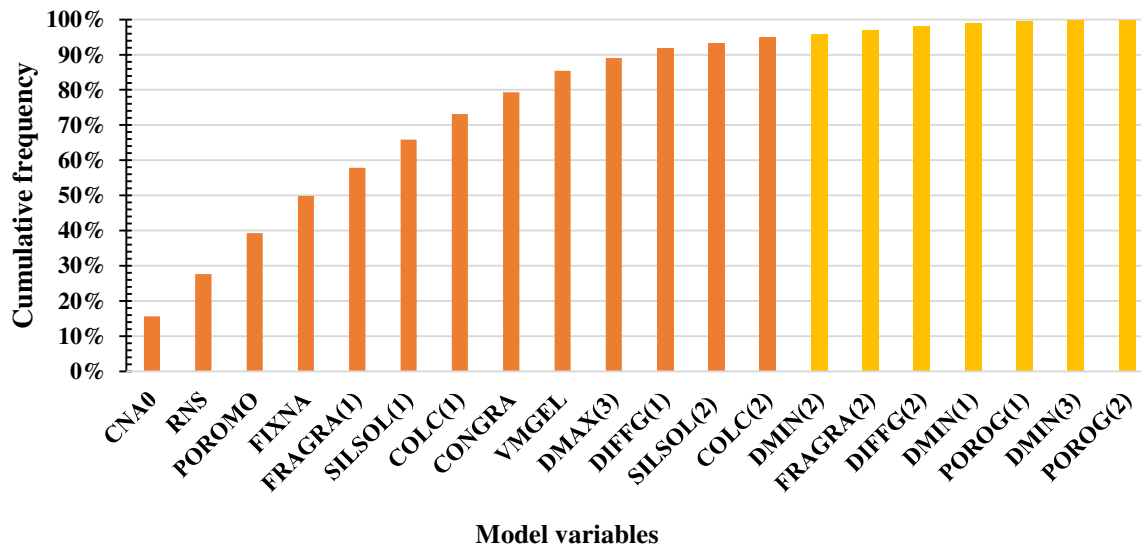
484 **Fig. 12.** Cumulative frequency on the sum of global sensitivity index of all outputs for a mean  
 485 elevated temperature (29 °C, representative of the structure core)

486 To be useful for other structures damaged by ASR in other locations in the world, the effect of the  
 487 temperature on the sensitivity of the model is secondly analysed on expansions evaluated for a  
 488 lower constant temperature of about 10 °C. In this case, the temperature is about 30 °C lower than  
 489 in the conditions of the expansion tests. A larger impact on the importance of each parameter can  
 490 be expected. Fig. 13 highlights the ranking modification of the parameters. For this low  
 491 temperature, the alkali concentration, CNA0, becomes the most important parameter and RNS, the  
 492 ratio of Na<sub>2</sub>O / SiO<sub>2</sub>, becomes the second most important parameter for the first time in all the  
 493 analyses.

494 The fixation of alkali, FIXNA, is still in fourth place. This confirms the importance of the kinetics  
 495 of reactive mechanisms for the modelling of ASR expansion even at low temperature. It is also  
 496 very interesting to note that, for low temperature, the reactive silica of the sand, SILSOL(1), is in  
 497 sixth place. While it was not a limiting parameter for the laboratory expansion test, the importance  
 498 of this parameter increases with decreasing temperature.

499

500



501

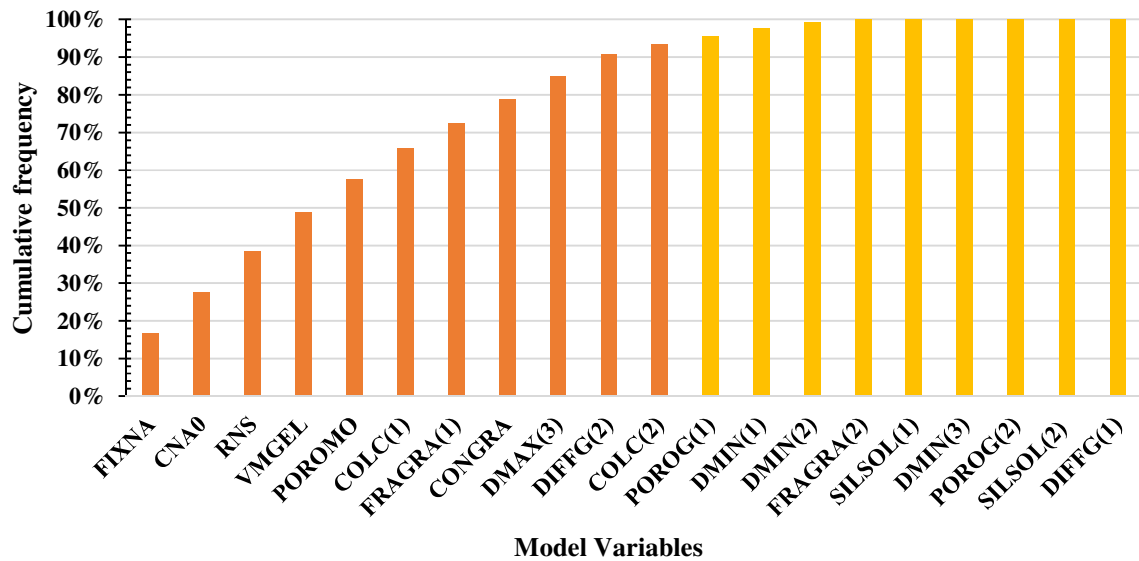
502 **Fig. 13.** Cumulative frequency on the sum of global sensitivity index of all outputs for a mean low  
 503 temperature (10 °C, representative of the structure core)

504

505 **5.3. Impact of variable temperature on the sensitivity**

506 In large engineering structures such as dams, the core of the structure is little impacted by  
 507 temperature cycles. Core temperature is almost constant. However, this is not the case for the skin  
 508 of structures. Expansions induced at the skin are important as they can lead to deformation  
 509 gradients and thus to cracking localized at the concrete skin. Such cracking can imply new paths  
 510 for water into the structures and can cause new water supply able to accelerate ASR and thus the  
 511 degradation of the structure.

512 Fig. 14 shows the cumulative analysis of the model for concrete subjected to the variable  
 513 temperature conditions, representative of the skin of Song Loulou dam.



514

515 **Fig. 14.** Cumulative frequency on the sum of global sensitivity index of all outputs for variable  
 516 temperature conditions (representative of the skin of Song Loulou dam)

517 As the variation of temperature in the course of the year is small for Song Loulou dam (about 5  
 518 °C), the impact on the analysis is small in comparison with the analysis performed for a constant  
 519 temperature of 29 °C (Fig. 12). All the 11 important variables are the same for the two analyses.  
 520 However, even this small modification can impact the relative ranking of these important  
 521 variables. For example, the mortar porosity, POROMO, passes from the third place to the fifth,  
 522 while the Na<sub>2</sub>O / SiO<sub>2</sub> ratio is more important for temperature cycling between 24 and 29 °C than  
 523 for the constant 29 °C. As the modification of kinetics with temperature follows an Arrhenius  
 524 exponential law, a small modification of temperature can lead to significant modifications of the  
 525 outputs.

526

527 **6. Discussion**

528 6.1 Lessons learnt for ASR modelling at material scale

529 For all the sensitivity analyses performed in this work, the parameter, FIXNA, which quantifies  
 530 the impact of reactive mechanisms on ASR kinetics is of prime importance, while the coefficients  
 531 of diffusion in the aggregate, DIFFG(i), seem to have little effect (except for the volume of gel,  
 532 V<sub>g</sub>, at 38 °C, Fig. 5 to Fig. 7). For all the situations, FIXNA is the most influential parameter,  
 533 except for expansion at low temperature (10 °C, Fig. 13 – but FIXNA is still ranked fourth).

534 This may seem surprising as a many models assume ASR kinetics to be controlled by alkali  
535 diffusion in the aggregate. It is known that this assumption is realistic for aggregates with fast  
536 reactivity, but not for certain slowly reacting aggregates, which present attacks distributed  
537 throughout the aggregate and not an attack localized at aggregate edges [18,44,61]. Both transport  
538 and the kinetics of chemical reactions have to be considered to obtain realistic representations of  
539 all types of reactive aggregate (slow or fast reacting particles) [28,39].

540 To interpret the results of this analysis and, in particular, the impact of the parameter FIXNA, it is  
541 important to note that the present study was carried out for data lying in the ranges found in  
542 existing literature and defined in Table 1. Thus, the coefficient of diffusion in aggregate was about  
543  $10^{-13}$  m<sup>2</sup>/s. It was measured through thin sections of quartzite aggregate in [47]. However, two  
544 points are open to discussion. Firstly, coefficients of diffusion in aggregate are probably very  
545 different from one rock to another (but few data on this type of measurements are available in the  
546 literature). Secondly, the principle of the diffusion measurement used in [47] is not fully  
547 representative of diffusion in ASR mechanisms: in [47], diffusion was evaluated through the time  
548 necessary for alkali to cross the sample. This crossing can be partly achieved through connecting  
549 paths. It does not mean that the aggregate is totally saturated in alkali. In the case of ASR, alkali  
550 has to reach all the reactive silica in the aggregate. As aggregates come from natural,  
551 heterogeneous material, diffusion is probably very different from one aggregate to another. The  
552 principle of measurement used in [47] evaluates the diffusion at macro-scale but the coefficient of  
553 diffusion in localized parts of the aggregate, representative of diffusion at micro scale, is probably  
554 smaller and very heterogeneous in the particles. This highlights the importance of having reliable  
555 experimental evaluations of all the parameters of the model if relevant sensitivity analysis is to be  
556 obtained.

557 Moreover, the expansions studied here were obtained on an aged concrete extracted from a thirty-  
558 year-old ASR-affected dam, while most of the ASR modelling in the literature is based on young  
559 concrete cast and kept in laboratory conditions. In our case, the aggregate attack was not  
560 homogeneous in the concrete at the beginning of the LPC N°44 accelerated test. In addition, as  
561 ionic diffusion is first necessary to cause the chemical attack (hydroxyl ions have to move to  
562 reactive silica to allow the dissolution), diffusion was probably more advanced than the chemical  
563 attack of aggregate at the beginning of the test. This could have modified the relative impact  
564 evaluated for the diffusion (DIFFG(i)) and the alkali fixation (FIXNA) on outputs during such  
565 tests, and could thus explain why the parameter FIXNA is so prominent in the present analysis.

566 The second fruitful lesson learnt concerning the modelling of ASR at material scale is the  
567 modification of the rank of parameters with the decrease of temperature. In particular, the  
568 increasing influence of RNS, the  $\text{Na}_2\text{O} / \text{SiO}_2$  ratio, with decreasing temperature should be noted.  
569 In this modelling, this ratio was not directly modified by the temperature (but, as temperature acts  
570 on equilibrium constants [27], this modification could improve the predictive capability of the  
571 model); only the kinetics parameters (FIXNA and DIFFG) were impacted by temperature in the  
572 present work. This means that the modification of the rank of RNS is a consequence of the  
573 combination of different equations. At 38 °C, the kinetics of diffusion is very high, thus a large  
574 proportion of the aggregates is rapidly saturated in hydroxyl and alkali. Ions are thus available in a  
575 sufficient number of locations to produce ASR gel and thus expansion. For lower temperatures,  
576 diffusion is slower. ASR gels can only be produced in a reduced number of locations. RNS, the  
577 ratio of  $\text{Na}_2\text{O} / \text{SiO}_2$ , drives the number of moles of ASR gels that can be produced in a particular  
578 location. One mole of  $\text{SiO}_2$  leads to 1 mole of ASR gel: if the RNS is high, the gel is richer in  
579 alkali. Alkali concentration has to be higher to produce the same quantity of gel. This is a  
580 collateral consequence of the decrease of the kinetics rate by temperature.

581 In this work, the sensitivity analysis focused on the physico-chemical part of ASR modelling and  
582 its impact of the kinetics of expansion. The mechanism of permeation of ASR gels through cracks  
583 is not considered. At material scale, swelling tests are affected by the loss of ASR gel through  
584 cracks resulting from expansion. Such loss of gels depends on the test temperature [62] but ASR  
585 modelling has to consider the mechanical consequences of ASR, and particularly the cracks, to be  
586 able to propose a reliable evaluation of this mechanism. In our approach, both ASR cracking and  
587 anisotropic effects due to stress would be considered at structural scale in other numerical ways.

588

## 589 6.2 Lessons learnt for reliability ASR modelling at structural scale

590 Sensitivity analysis can be used to detect the most influential parameters for material modelling  
591 and thus decrease the number of inputs if their impact is minimal. When structural modelling is  
592 employed in a probabilistic context, only the major influential parameters have to be considered  
593 random. The other parameters can be considered as deterministic since they have little influence  
594 on the variability of outputs. This can help to avoid time-consuming calculations. Thus, resources  
595 and efforts can be concentrated on improving the knowledge of leading parameters.

596 Combined analyses performed in the present paper point out that almost 60% of the parameters of  
597 the model have significant influence on the results considering five outputs. For some particular

598 sensitivity analyses (gel volume or expansion), only 30% of the parameters have important effects.  
599 For structural analysis, it is thus important to determine the most prominent outputs in order to  
600 decrease the number of random parameters.

601 Temperature modifies the relative importance of ASR modelling parameters. For structural  
602 condition assessment, some parameters can be calibrated on laboratory tests performed at 38 °C,  
603 while the damaged structure is usually exposed to lower and fluctuating temperatures.  
604 Consequently, the number of random parameters (the most influential ones) is increased for ASR  
605 modelling for reliability in field conditions.

606 For the analysis of concrete already damaged by ASR (case of condition assessment of damaged  
607 structures), 3 parameters amongst the most influential ones are the same for all the environmental  
608 conditions: the coefficient of alkali fixation (FIXNA), the initial alkali concentration (CNA0) and  
609 the porosity of the cement paste (POROMO). The molar volume of gel (VMGEL) and the reaction  
610 rim thickness for small aggregates (COLC(1)) have major impacts on the output for laboratory  
611 tests, while the ratio of Na<sub>2</sub>O / SiO<sub>2</sub> of ASR gels (RNS) has a major impact in the temperature  
612 conditions of Song Loulou dam. All these six parameters, at least, should be considered as random  
613 for the reliability analysis of Song Loulou dam. For lower temperature, the fraction of the smallest  
614 granular class of aggregates (FRAGRA(1)) also has an important impact (Fig. 13).

## 615 **7. Conclusion**

616 A sensitivity analysis using the Morris method based on the ASR model developed at the material  
617 scale in LMDC was carried out to reduce the stochastic dimension for a further reliability analysis.  
618 Five outputs of the model were targeted: the total volume of gel, the ASR expansions, the  
619 expansion rate, the advancement of ASR in terms of expansion and the time to reach this  
620 advancement. A method to determine the most important parameters for multiple outputs using the  
621 cumulative frequency of the sum of global sensitivity indices on all the outputs has been proposed  
622 and applied not only time-wise but also over several times. Parameters were selected with a  
623 cumulative frequency using a threshold value of 95%. Whatever the conditions, 60% of the  
624 parameters have a major influence on all the outputs while only 30% of parameters affect a  
625 particular output.

626 The parameters underlined as the most relevant in this sensitivity analysis are known to affect  
627 ASR kinetics and expansion, even if they are not always taken into account in the models found in  
628 the literature. In particular, the kinetics of reactive mechanisms are often ignored by models at the  
629 material scale. This sensitivity study has shown that this may jeopardize the accuracy of the results

630 if they are used to analyse the expansion of cores drilled from damaged structures like the ones  
631 used in the present work (coming from Song Loulou dam). It is also important to note the  
632 dependency of the influential parameters on the temperature. The most significant parameters are  
633 not the same for laboratory expansion tests at 38 °C and for real structures under low  
634 temperatures. This points out the impact of the mechanisms quantified by these parameters and  
635 their relative role according to temperature. A mechanism that is important at 38 °C can be  
636 negligible at 10 °C. This explains why it is often so difficult to translate a conclusion obtained in  
637 laboratory conditions to real structures.

638 In a probabilistic context, where the reliability analysis of dams exposed to ASR has to be  
639 conducted, only the major parameters should be considered random for structural calculations.  
640 The major parameters have to be determined for both temperatures if the model is calibrated on  
641 laboratory tests and then used for structural assessment in field conditions. Future work should  
642 assess the dam reliability [50].

643

#### 644 **Credit authorship contribution statement**

645 **G. Ftatsi Mbetmi:** Conceptualization, Methodology, Programming, Results discussion, Writing –  
646 original draft, Writing - review & editing. **S. Multon:** ASR modelling expertise, Methodology,  
647 Results discussion, Writing - review & editing. **T. De Larrard:** Conceptualization, Methodology,  
648 Results discussion, Writing - review & editing. **F. Duprat:** Conceptualization, Methodology,  
649 Results discussion, Writing - review & editing, Supervision. **D. Tieudjo:** Writing - review &  
650 editing, Supervision, computing resources.

#### 651 **Declaration of competing interest**

652 None of the five authors have a conflict of interest.

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**Input:**  $k$ , number of input variables ;  $X_{min}^i$  and  $X_{max}^i$ , minimum and maximum values of variables  $X_i$  with  $i = 1, \dots, k$  ;  $p$  with  $p > k$ , the number of levels of each variation range;  $r$ , the number of trajectories,  $S_{thv}$ , sensitivity threshold value.

**Output:** Important variables

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**Begin**

Initialize the lower triangular matrix  $B_{(k+1) \times k}$

Initialize the matrix  $J_{(k+1) \times k}$  of  $(k+1)$  lines and  $k$  columns, of ones

Initialize the diagonal matrix  $D_{k \times k}^*$  whose diagonal terms randomly take the values 1 or -1

Initialize the matrix  $P_{k \times k}^*$  such that each column and each line contain only one element equal to 1 and the others are equal to 0

Compute  $\Delta = \frac{1}{p-1}$

Construct the levels vector  $Vn[l] = \frac{l-1}{p-1}, l = 1, \dots, p$

**for**  $m=1$  **to**  $r$  **do**

For each variable, randomly draw a value of  $Vn$  ; the set of  $k$  values obtained constitute the vector  $X_{1 \times k}^*$  of the coordinates of the initial point in the standard space.

Compute  $B_{(k+1) \times k}^*$  using (Eq.4)

Compute  $X^{j,i}, i = 1, 2, \dots, k; j = 1, 2, \dots, k + 1$  using (Eq.5)

Compute  $f(X_i)$  of each of  $k + 1$  points of the trajectory

Compute the elementary effects,  $EE_i = \frac{f(X_{i+1}) - f(X_i)}{\Delta}, i = 1, 2, \dots, k$

**end for**

Compute the absolute means on  $r$  of the  $EE_i, \mu_i^*$

Compute the means and standard deviation on  $r$  of the  $EE_i, \mu_i$  and  $\sigma_i$

Compute the global sensitivity indices of each variable,  $S_i^*$  using (Eq.7)

**if** single output

Order  $S_i^*$  decreasingly and cumulate

Select variables with a cumulative  $S_i^*$  less than  $S_{thv}$

**else**

For each variable, sum  $S_i^*$  on all outputs

Compute the frequencies on  $\sum S_i^*$ , order decreasingly, and cumulate

Select variables with cumulative frequencies less than  $S_{thv}$

**end if**

**End**

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