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► **To cite this version:**

Stéphane Multon, Alain Sellier, Martin Cyr. Chemo-mechanical modeling for prediction of alkali silica reaction (ASR) expansion. *Cement and Concrete Research*, 2009, 39 (6), pp.490–500. 10.1016/j.cemconres.2009.03.007 . hal-01724667

HAL Id: hal-01724667

<https://insa-toulouse.hal.science/hal-01724667v1>

Submitted on 20 Feb 2019

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Chemo-mechanical modeling for prediction of alkali silica reaction (ASR) expansion

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Abstract

The effect of the size of the aggregate on ASR expansion has already been well illustrated. This paper presents a microscopic model to analyze the development of ASR expansion of mortars containing reactive aggregate of different sizes. The attack of the reactive silica by alkali was determined through the mass balance equation, which controls the diffusion mechanism in the aggregate and the fixation of the alkali in the ASR gels. The mechanical part of the model is based on the damage theory in order to assess the decrease of stiffness of the mortar due to cracking caused by ASR and to calculate the expansion of a Representative Elementary Volume (REV) of concrete. Parameters of the model were estimated by curve fitting the expansions of four experimental mortars. The paper shows that the decrease of expansion with the size of the aggregate and the increase of the expansion with the alkali content are reproduced by the model, which is able to predict the expansions of six other mortars containing two sizes of reactive aggregate and cast with two alkali contents.

Keywords: alkali-silica reaction (ASR), particle size, alkali content, expansion, model

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27 **1. Introduction**

28 Alkali Silica Reaction is a chemical reaction between the alkalis of cement and the reactive
29 silica of concrete structure aggregates. The reaction products are expansive gels which induce
30 stresses, and hence cracking, in concrete. The main research on ASR concerns the expert
31 appraisal of damaged structures [1-5]. Modeling ASR and the resulting expansion is
32 necessary to obtain relevant predictions of the structural responses of damaged structures and
33 models must take the chemical and physical aspects into account.

34 The LMDC (Laboratoire des Matériaux et Durabilité des Constructions), with EDF
35 (Electricité de France) as a partner, has been working to establish a general method for the
36 reassessment of ASR-damaged structures. The method uses expansion measurements on
37 small specimens (2 x 2 x 16 cm) of mortar cast with crushed aggregates extracted from
38 damaged structures [6-7] in order to evaluate the advancement of the reaction on the
39 aggregates. As shown in [6-7], the advancement varies with the size of the aggregates because
40 of the time taken for alkali to diffuse into the aggregate. One of the advantages of this method
41 is that it performs calculations by using the state of advancement of the different aggregate
42 sizes in the structure concrete, which allows relevant predictions to be obtained. However,
43 this research needs to be completed by the development of microscopic modeling that uses the
44 tests proposed in [6-7] in a reliable way, particularly according to the effect of the alkali
45 content and the size of the reactive aggregate particles on the ASR-expansions. Predicting the
46 expansion of concrete in real damaged structures is the final aim of this model. However, as a
47 first step, it is used here to analyze laboratory experiments where the effects of mechanical
48 stresses and environmental conditions on expansion are not considered. Similarly, alkali
49 regeneration by calcium ions, which is a slow process [8-10], is not taken into account.

50 This paper deals with the development of an empirical microscopic ASR model. The main
51 input data to such models are alkali and reactive silica contents, aggregate sizes, and
52 mechanical properties of the mortar. The main result is the prediction of the ASR expansion
53 of the concrete taking into consideration the physicochemical mechanisms of the reaction.
54 Among the existing microscopic ASR models, some were developed to take the mechanics of
55 ASR into consideration [11-12], and others focus on the chemical phenomena [13]. Finally,
56 some models take both aspects into account [14-18]. Many phenomena of ASR can be
57 described by the existing models (e.g. diffusion of alkali into the aggregates, gel permeation
58 and imbibition); but others cannot be correctly represented yet (e.g. evolution of the
59 concentration of alkali during the reaction, and expansion of concrete containing different
60 sizes of reactive aggregate).

61 The microscopic model developed in this paper is based on some of these previous models
62 [13-14, 17-18]. It can predict the damage and the expansion of a Representative Elementary
63 Volume (REV) of concrete containing a mix of reactive aggregates of different sizes. The
64 diffusion of alkali into the aggregate is taken into account; the production of the ASR gel
65 increases with the molar concentration of alkalis in the aggregate. In the cement paste
66 surrounding the reactive aggregate, the concentration of alkalis decreases with their diffusion
67 towards the aggregate and their consumption by the ASR gel. The gel permeates into a part of
68 the porous volume connected to the reactive aggregate. Once the available porous volume has
69 been filled by the gel, the pressure due to ASR acts on the surrounding cement paste, leading
70 to damage and expansion.

71 The modeling principles and assumptions are first presented and discussed. Then, the
72 physicochemical and mechanical models are developed in two parts. Finally, the model is
73 used to calculate the expansion of ten mortars containing different amounts of two sizes of
74 reactive aggregate and having two alkali contents. Five parameters of the physicochemical

75 model cannot be obtained by direct measurements and are therefore calculated by inverse
76 analysis using four of the ten mortars. The parameters thus obtained are used to predict the
77 expansions of the other six mortars. Once the mechanical characteristics of the sound concrete
78 are known, no additional fitting of parameters is necessary for the mechanical modeling. The
79 last part points out the qualities and the limitations of the model and gives some indications as
80 to how it could be improved.

81 **2. Principles**

82 ***2.1 Physicochemistry and mechanics of ASR***

83 As in previous works [13,15,18], the model developed in this paper used the reaction
84 mechanisms presented by Dent Glasser and Kataoka [19]:

85 - The first part of the reaction is the diffusion of the alkali and hydroxyl ions into the reactive
86 aggregate, and the destruction of the silanol and siloxane bonds contained in the reactive
87 silica.

88 - The second part is the formation of the ASR gels in presence of water and calcium ions [19-
89 21]. Once formed, the gel permeates through a part of the connected porous volume between
90 aggregate and cement paste and fills a part of the connected porosity [22]. Then the gel exerts
91 a pressure on the cement paste, which causes cracking and expansion of the concrete.

92 Moreover, in order to complete the physical considerations, assumptions based on numerous
93 experimentations already published were made: the existence of a threshold in alkali
94 concentration under which ASR does not occur [23-26], the high nonlinearity of the
95 dissolution of the reactive silica with pH [29] and the stoichiometry of ASR gels [30-32].

96 **2.2 Assumptions**

97 It is not possible to consider all the physical and chemical mechanisms of such a reaction
 98 occurring in a complex medium like concrete. Simplifications have to be assumed in order to
 99 model ASR expansion in accordance with most phenomena.

100 **2.2.1 Geometry**

101 The reactive aggregate and the Relative Elementary Volume (REV) of concrete surrounding
 102 the reactive aggregate are assumed to be spherical (Figure 1).

103

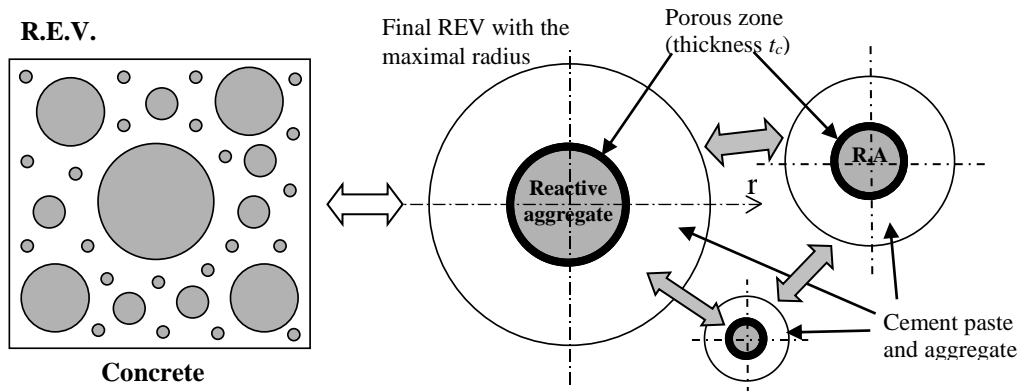


Figure 1 – Definition of the Relative Elementary Volume for several reactive aggregate sizes [18]

104

105 The radius of the REV depends on the radius and the content of the reactive aggregate in
 106 concrete, as given by equation 1 [18]:

$$R_{REV}^a = \frac{R_a}{\sqrt[3]{\phi_a \cdot C_{agg}}} \quad (1)$$

107 with:

108 a , a superscript relative to the size fraction of the reactive aggregate with mean radius R_a

109 R_{REV}^a the REV radius corresponding to the aggregate size fraction a

110 ϕ_a the volume fraction of reactive aggregates with mean radius R_a

111 C_{agg} the volume fraction of all the aggregate per m^3 of concrete.

112 The number of reactive aggregates per m^3 of concrete N_a is equal to:

$$N_a = \frac{\phi_a \cdot C_{agg}}{\frac{4}{3} \pi R_a^3} \quad (2)$$

113 2.2.2 Diffusion of alkali and attack of reactive silica

114 In the model presented in [18], the diffusion of the ionic species into both reactive aggregate
115 and cement paste surrounding the aggregate is considered. However, at each time step, the
116 concentrations of ionic species are roughly homogeneous in the cement paste. This can be
117 explained by the differences between the coefficients of diffusion in the cement paste (about
118 $10^{-11} m^2/s$) and in the aggregate (about $10^{-15} m^2/s$). Thus, diffusion into the cement paste
119 appears to be instantaneous compared to diffusion into the aggregate, so the alkali
120 concentration was assumed to be uniform in the paste in the present model. This constitutes
121 the main simplification in relation to Poyet's modeling [18].
122 Moreover, the aggregate was taken as spherical. Thus the concentrations of the ionic species
123 diffusing into the aggregate depend only on the time and on the radius r from the centre of the
124 reactive aggregate (Figure 2).

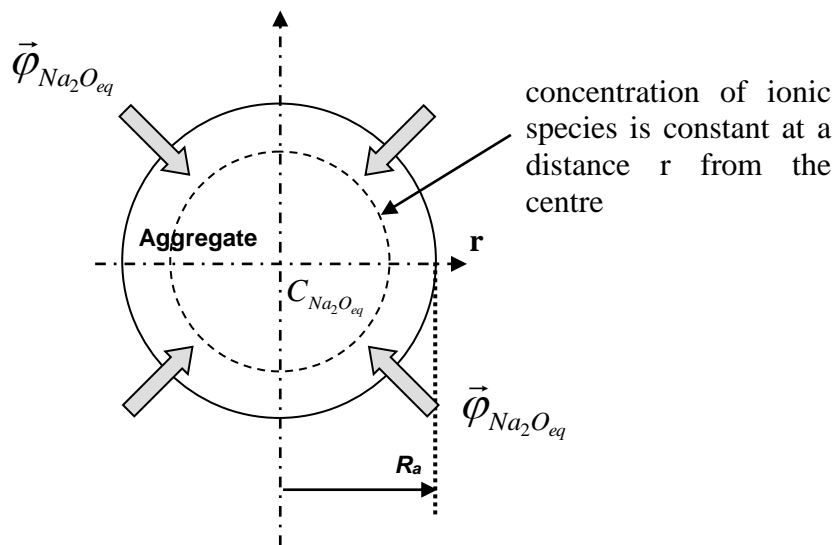


Figure 2 – Diffusion of Na_2O_{eq} in aggregate

125

126 Several authors showed that no expansion occurred in concrete containing alkali silica
127 reactive aggregate for low alkali contents: under a threshold lying between 3 and 5 kg/m³ [23-
128 26] or for an alkali concentration lower than 0.5 or 0.6 mol/l of Na⁺ [27-28]. Urhan reports that
129 the solubility of silica is quite constant in a solution having a pH of less than 9 or 10 but
130 increases rapidly for higher pH [29]. Due to the high nonlinearity between the pH and the
131 solubility of the silica and to the relationship between the value of the pH in a solution and the
132 concentration of alkali, the destruction of the reactive silica was assumed to increase
133 significantly when the concentration of alkalis in a part of the aggregate was higher than a
134 threshold concentration noted Na_{th} . When the threshold is reached and passed, the present
135 model assumes that gel formation increases with a rate proportional to the difference between
136 the alkali concentration in the aggregate and the threshold. The same rate is taken for the
137 alkali consumption by the ASR gels. Therefore, the kinetics of the reaction, and thus of the
138 gel formation, is assumed to be controlled by the destruction of the reactive silica due to alkali
139 diffusion. Some authors [8-10] consider that the gel formation depends on the presence of
140 calcium ions. This has not been taken into account in the model. However, as calcium is
141 provided by portlandite dissolution and as this dissolution is not possible while the alkali
142 content is high, the need for calcium can be neglected during the first step of an accelerated
143 test. This aspect of the reaction will have to be carefully considered for the simulation of
144 long-term ASR phenomena. So the extension of the present model to structural applications
145 will have to include calcium substitution.

146 **2.2.3 ASR gel**

147 Another problem for ASR modeling concerns the assumptions on the compositions of the gels
148 produced by the reaction. The compositions of the gels depend on many parameters, such as
149 gel position in the concrete (in or out of the aggregate) and its age (it is usually assumed that
150 old gels contain more calcium than new). The Na₂O / SiO₂ ratio in the gels varies from about

151 0.1 to 0.4 [30-32]. It is quite difficult to obtain a relevant and representative value for the gel
 152 composition. In the model presented here, the Na₂O / SiO₂ ratio is assumed to be equal to the
 153 mean value 0.2 obtained in laboratory experiments in [32]; it is assumed that 1 mole of
 154 Na₂O_{eq} reacts with 5 moles of SiO₂ to give 1 mole of ASR gel. The volume of gel produced
 155 by one size of aggregate n_g^a is obtained by multiplying the number of moles of ASR gel
 156 produced by the aggregate a by the molar volume of the gel V_{gel}^{mol} (in m³/mol). The total
 157 volume of gel formed is then the sum of the volume of gel produced by all the aggregates (in
 158 m³):

$$V_g = \sum_i n_g^a \times V_{gel}^{mol} \quad (3)$$

159 As described just above, after its formation, the gel can permeate through a part of the
 160 connected porous volume surrounding the aggregate [33] or can stay in the cracks of the
 161 aggregate. This part of connected porosity is modeled as a volume of porosity totally filled by
 162 the gel with an equivalent thickness t_c (Figure 1, Eq 4). The equivalent thickness is assumed
 163 not to change with the size of the aggregate. Thus, the volume of gel necessary to fill this
 164 porosity, which consequently which does not exert pressure, is equal to the connected
 165 porosity (p):

$$V_{por} = \frac{4}{3} \pi \left((R_a + t_c)^3 - R_a^3 \right) p \quad (4)$$

166 The larger the aggregate size, the lower the ratio ‘connected porous volume / aggregate
 167 volume’. Therefore the largest aggregate causes the largest ASR-expansion.

168

169

170

171 **2.2.4 Mechanical considerations**

172 The model is supposed to calculate ASR expansion for stress free specimens. Moreover, the
173 mechanical properties are taken to be isotropic and, thus, the mechanical behavior of the
174 aggregate and of the cement paste in the REV is taken as isotropic. The behaviors of the two
175 media are assumed to be elastic for stresses lower than their compressive and tensile
176 strengths. The expansions due to ASR occur over long periods. During the process, the
177 materials are not subjected to instantaneous loading but to progressive stresses which cause
178 creep strains in the concrete [5]. In order to take the effect of concrete creep on the ASR
179 expansion into account, the calculations are performed with a long-term Young's modulus
180 equal to a third of the instantaneous Young's modulus (which is the usual value used in the
181 French reinforced concrete design code [34]). For the same stress, using the long-term
182 modulus rather than the instantaneous modulus leads to larger strains. The strains are then
183 equal to the sum of the instantaneous strains due to the ASR gel pressure and the creep strains
184 of the cement paste under the ASR gel pressure. If the stresses become higher than the tensile
185 strengths of the materials, cracking and damage occur in the concrete. In the following
186 calculations, the crack density is consistent with the damage to the concrete calculated by the
187 model (the damage is defined as the decrease of the long-term Young's modulus due to
188 cracking). After cracking, the gel is assumed to permeate into the cracks.

189

190 **3. Physicochemical modeling**

191 The physicochemical modeling concerns the diffusion of the alkali ions into the aggregate and
192 the formation of the ASR gel. The alkali diffusion into the aggregate is controlled by the mass
193 balance equation with a depletion term to represent the consumption of alkali during the
194 formation of the ASR gel. The volume of gel produced by the reaction can then be calculated
195 from the alkali consumed in the mass balance equation. The equations are solved numerically
196 by using a geometrical discretization based on finite volumes and time discretization by
197 Euler's method.

198 **3.1 Mass balance equation**

199 **3.1.1 Alkali diffusion in aggregate**

200 Just after casting, the alkali concentration is high in the cement paste and negligible in the
201 aggregate. Therefore, a flux of alkali (Na^+ and K^+) appears between the cement paste and the
202 core of the aggregate. The mass balance of alkali in the aggregate with the assumed spherical
203 symmetry can be described by the equation:

$$\frac{\partial}{\partial t} (p_{agg} S_r C_{Na}) = \frac{1}{r^2} \frac{\partial}{\partial r} \left(D \cdot r^2 \frac{dC_{Na}}{dr} \right) + S(C_{Na}) \quad (5)$$

204 with:

205 t the time

206 p_{agg} the porosity of the aggregate,

207 S_r the saturation degree,

208 C_{Na} the concentration of alkali (Na^+ and K^+),

209 r the distance from the center of the aggregate,

210 D coefficient of diffusion of alkalis into the aggregate,

211 and $S(C_{Na})$ the depletion term that represents alkali consumption.

212 In order to solve the equation, two boundary conditions were used:

213 - at the centre of the aggregate ($r=0$), the flux is equal to zero;

214 - at the external boundary ($r=R_a$), the alkali concentration is equal to C_{Na}^{cp} , the alkali

215 concentration in the cement paste. For the initial condition, this concentration is equal to:

$$C_{Na}^{cp} = 2 \times \frac{M_{Na2O}}{M_{Na2O}^{mol}} \times \frac{1}{p_{cp} S_r (1 - C_{agg})} \quad \text{with } p_{cp} = \frac{p_{mort} - p_{agg} \cdot C_{agg}}{(1 - C_{agg})} \quad (6)$$

216 with:

217 M_{Na2O} the mass of equivalent alkali per m^3 of concrete,

218 M_{Na2O}^{mol} the molar mass of equivalent alkali (equal to 0.062 kg/mol),

219 p_{cp} , p_{mort} , p_{agg} the porosity of the cement paste, mortar, and aggregate respectively,

220 and C_{agg} the aggregate concentration per m^3 of concrete.

221 During the process, the concentration of alkali in the cement paste decreases due to alkali

222 diffusion into the aggregate (see next part).

223 3.1.2 Alkali concentration in the cement paste

224 The variation of alkali content in the cement paste is due to the diffusion from the paste to the

225 aggregate. It is equal to the sum of the flux of alkali at the boundary ($r=R_a$) between all the

226 aggregate and the paste. For concrete containing several size fractions, a , of reactive

227 aggregate, the flux has to be summed over all of them. It can be calculated by:

$$\frac{\partial}{\partial t} (p_{cp} S_r C_{Na}) = \sum_a N_a \cdot D \cdot 4\pi R_a^2 \frac{dC_{Na}^a}{dr} (R_a) \quad (8)$$

228 with N_a the number of reactive aggregates (Eq 2).

229 3.1.3 Consumption of alkalis

230 As explained in the 'Assumptions' section, the consumption kinetics of alkalis is assumed to

231 be proportional to the difference between the concentration of alkali in the aggregate and the

232 threshold above which the silica dissolution starts. Thus, the depletion term of the mass
 233 balance equation is:

$$S(C_{Na}) = f \langle C_{Na} - Na_{thr} \rangle^+ \quad (9)$$

234 With: f , the alkali fixation coefficient. This is the coefficient of proportionality between the
 235 consumption kinetics of alkali and the difference between the concentration of alkali in the
 236 aggregate and the alkali threshold. f is a negative parameter. Note that it could depend on the
 237 temperature if AAR dependence on temperature is to be modeled.

238 $\langle X \rangle^+$ is equal to X if $X > 0$ or equal to 0 if $X \leq 0$.

239 $S(C_{Na2O})$ is the amount of alkali fixed per m^3 of aggregate. If the concentration of alkalis in
 240 the aggregate is lower than the alkali threshold, the term is zero; there is no consumption of
 241 alkali and no ASR-gel formation. If the concentration is higher than the threshold, the
 242 consumption of alkali starts with the kinetics given by equation 9.

243 Moreover, the consumption of alkali has to be stopped when all the reactive silica contained
 244 in the aggregate has reacted with alkali. As the Na_2O / SiO_2 ratio of the gel is assumed to be
 245 equal to 0.2 [32], the end of the alkali fixation is obtained when the amount of alkali fixed by
 246 the aggregate is equal to 0.2 times the reactive silica content of the aggregate.

247 Note: The unit of the alkali fixation coefficient is (mol/ m^3 of aggregate) per (mol/ m^3 of
 248 solution) per second.

249 **3.2 Formation of the ASR gel**

250 The number of moles of ASR gel produced in the aggregate a at time step t is equal to the
 251 number of moles of Na_2O consumed by the reaction, thus half the number of moles of Na^+ :

$$n_g^a = \frac{4}{3} \pi R_a^3 \times \int_0^t \frac{S(C_{Na})}{2} dt \quad (10)$$

252 Finally, the volume of gel produced by the reaction is given by the Equation 3.

253 **4. Mechanical modeling**

254 The main result of the chemical modeling is V_g , the volume of ASR gel formed by the
255 reaction. The volume of gel is then used to determine the strain induced on the REV and
256 finally the expansion of the damaged concrete caused by the chemical reaction. As for the
257 chemical modeling, the equations of mechanical equilibrium are calculated on the spherical
258 REV, as has already been described for elastic conditions in [11,14,17]. In the REV, the
259 mechanical equations are used for two media: a , the aggregate under study, and SC , the
260 concrete surrounding the studied aggregate (medium including cement paste and other
261 aggregate – Figure 3). The cracking due to ASR is taken into account by isotropic mechanical
262 damage [35-36]. Thus, the mechanical problem is assumed to be non-linear elastic due to the
263 introduction of the damage variable. The equations developed below present an analytical
264 solution and are applied to each aggregate size.

265 **4.1 Strain-stress equations**

266 The ASR gel is supposed to be incompressible compared to the elastic properties of the
267 cement paste and aggregate. Therefore, the ASR expansion can be taken into account as an
268 imposed strain in the aggregate elastic constitutive law:

$$\underline{\underline{\sigma}}_a = \lambda_a \text{tr} \underline{\underline{\varepsilon}}_a \cdot \underline{\underline{I}} + 2 \cdot \mu_a \cdot \underline{\underline{\varepsilon}}_a - (3\lambda_a + 2\mu_a) \cdot \underline{\underline{\varepsilon}}_{\text{impl}}(t) \quad (11)$$

269 The constitutive law of the medium SC only considers the elastic effect of the material:

$$\underline{\underline{\sigma}}_{SC} = \lambda_{SC} \text{tr} \underline{\underline{\varepsilon}}_{SC} \cdot \underline{\underline{I}} + 2 \cdot \mu_{SC} \cdot \underline{\underline{\varepsilon}}_{SC} \quad (12)$$

270 with

271 $\underline{\underline{\sigma}}$ the stress matrix for each material,

272 $\underline{\underline{\varepsilon}}$ the strain matrix for each material,

273 $\underline{\underline{I}}$ the unit matrix,

274 λ and μ are, for each material:

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \text{ and } \mu = \frac{E}{2(1+\nu)} \quad (13)$$

(14)

275 where E is the Young's modulus and ν , the Poisson's coefficient of the medium.

276 ε_{impl} is the imposed strain applied to the aggregate.

277 The imposed strain applied to the aggregate is isotropic. It is assessed from the increase in
278 volume due to gel formation; the details of the calculation are given below (Equation 23).

279 The displacements in the materials are deduced by solving the equilibrium equation of the
280 elastic solids $\underline{\underline{div\sigma}} = 0$ assuming spherical symmetry. Displacements u_a in the aggregate and
281 u_{SC} in the surrounding concrete then depend only on the radius r :

In the aggregate a :
$$\underline{u}_a(r) = A_a \cdot r \cdot \underline{e}_r \quad (15)$$

In the surrounding concrete SC :
$$\underline{u}_{SC}(r) = \left(A_{SC} \cdot r + \frac{B_{SC}}{r^2} \right) \cdot \underline{e}_r \quad (16)$$

282 The three unknown constants (A_a , A_{SC} and B_{SC}) are determined from the following
283 boundary conditions (Figure 3):

- 284 - The radial displacements at the boundary between the aggregate and the surrounding
285 concrete are equal;
- 286 - The radial stresses are continuous at the boundary between the aggregate and the
287 surrounding concrete;
- 288 - The radial stress on the external surface is equal to zero (unloaded REV) (note: this
289 assumption leads to a free swelling model).

290 The mechanical equations can thus be solved and the variation of the stresses in the two
291 media can be analyzed. Due to the gel swelling, the aggregate is subjected to an isotropic
292 stress (pressure). This pressure is balanced by radial compressive stress in the concrete

293 surrounding the aggregate (decreasing from the aggregate pressure (at R_a) to zero on the REV
 294 external surface), and tensile stress in the tangential directions. The variation of the tensile
 295 stress in the tangential directions $\sigma_{\theta\theta}$ and $\sigma_{\varphi\varphi}$ with the radius has been plotted in Figure 3.

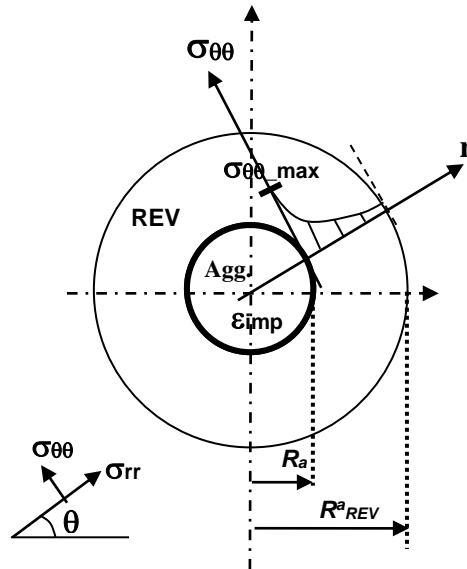


Figure 3 – Tensile stress in the REV subjected to ASR induced strains

296
 297 The maximum tensile stress is located at the boundary between the aggregate and the
 298 surrounding concrete. As the strength of concrete is higher in compression (f_c) than in tension
 299 (f_t), radial cracks due to the tensile stresses appear first and damage the surrounding concrete
 300 zone between the aggregate (R_a) and a radius R_d ($R_d - R_a$ corresponds to the crack length). In
 301 the following section, the damage theory is used to replace the cracked concrete by an
 302 equivalent concrete with a reduced Young's modulus. This modeling has the advantage of
 303 leading to an equivalent elastic problem, governed by the same set of equations as the
 304 previous ones, but with a lower Young's modulus.

305 **4.2 Damaged REV**

306 **4.2.1 Damaged Young's modulus of the REV**

307 The REV contains several reactive aggregates (Figure 1), which all cause cracks in the REV.
308 The interactions between the cracks of the different aggregates in the REV cause a decrease in
309 the concrete modulus. This can be modeled by a damage variable [35]. The damage
310 evaluation method is based on the strain equivalence principle [36]: the cracked medium
311 (initial Young's modulus E_0) is replaced by an equivalent medium without cracks but with a
312 lower modulus E_d (Figure 4) leading to the same displacement as the cracked one with the
313 initial Young's modulus.

314

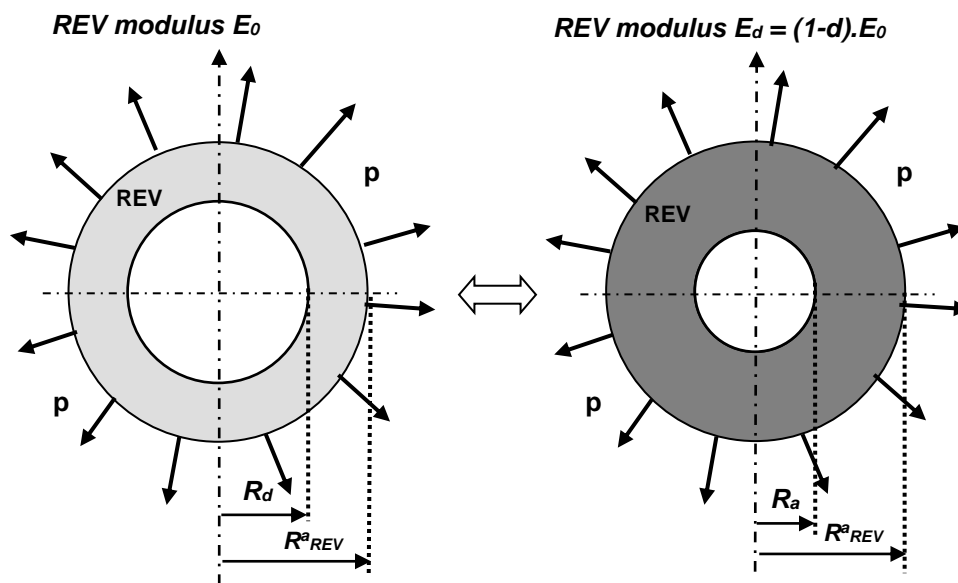


Figure 4 – Determination of the modulus of the damaged concrete

315

316 Therefore, as the cracked zone cannot withstand radial tension exceeding the tensile strength,
317 the residual uncracked surrounding concrete is equivalent to a hollow sphere with inner and
318 outer radii equal to R_d and R^a_{REV} under pressure p . According to the strain equivalence
319 principle, the radial strain of this hollow sphere must be equal to the radial strain of the

320 uncracked hollow sphere with inner and outer radii equal to R_a and R_{REV}^a under pressure p but
321 with a damaged Young modulus E_d (Figure 4). The damaged variable is then defined by:

$$d = 1 - \frac{E_d}{E_0} \quad (17)$$

322 Thus, the first hollow sphere, with a modulus of E_0 , and the second one, with a modulus of $(1-$
323 $d)E_0$ (Figure 4), have the same stiffness. If the inner radius R_d of the first sphere is equal to R_a ,
324 the strain of the cracked medium is equal to the strain of the medium without cracks and the
325 damage d is equal to 0. If the inner radius R_d of the first sphere becomes close to the outer
326 radius R_{REV}^a , the strain of the cracked medium increases and the damage d increases towards
327 1. Calculations are successively performed for all the aggregate size fractions a , and the
328 maximum value of damage is used to determine the modulus of the equivalent medium E_d :

$$E_d = (1 - d)E_0 \quad (18)$$

329 **4.2.2 Evaluation of the REV expansion**

330 Finally, the mechanical problem studied to assess the ASR-expansion is presented in Figure 5.
331 As explained above, the model assumes that the cracks close to the aggregate are filled by the
332 ASR gels. Thus, three parts can be distinguished (Figure 5): the central aggregate (between
333 radii 0 and R_a), the cracked zone filled by the gel (between radii R_a and R_{cz}) and the part of the
334 REV not yet cracked.

335

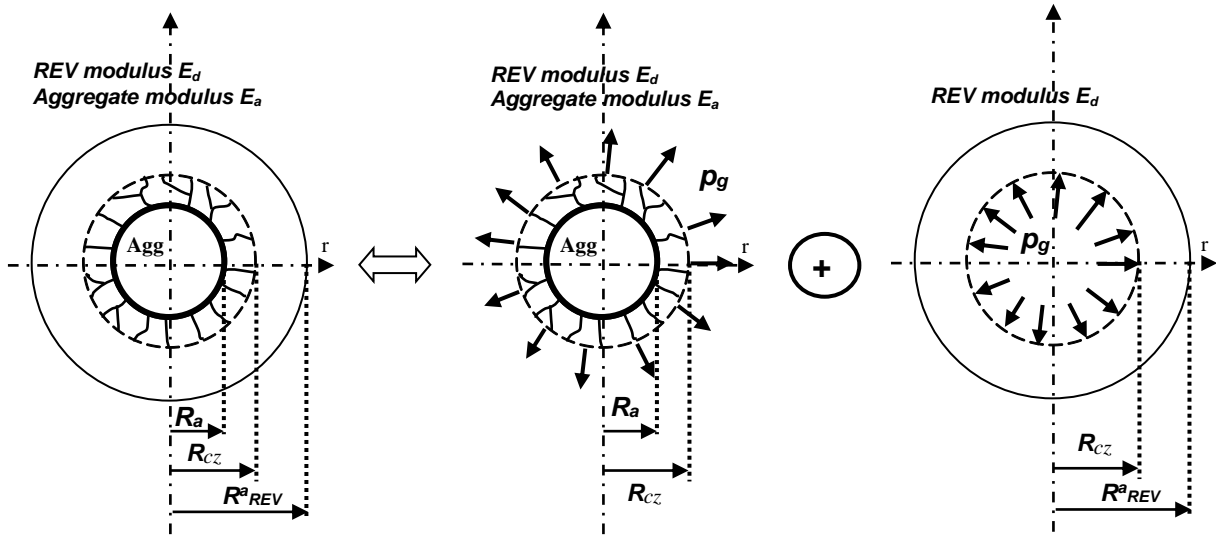


Figure 5 – Mechanical equilibrium of the damaged REV

336

337 As the gel reaches the cracks connected to the reactive aggregate, the radius R_{cz} corresponds
 338 to the radius R_d used to determine the damage (Figure 4). The gel pressure is constant in both
 339 the aggregate and the cracked zone; it is then applied to the internal boundary of the
 340 surrounding uncracked concrete. The modulus of the whole medium surrounding the
 341 aggregate is equal to E_d according to the damaged Young's modulus evaluated just above.
 342 The following behavior equation, concerning the part of the REV surrounding the aggregate
 343 and filled by the ASR gel, had to be added:

344 - the constitutive law:

$$\underline{\underline{\sigma_{cz}}} = \lambda_{fg} tr \underline{\underline{\varepsilon_{cz}}} \cdot \underline{\underline{I}} + 2 \cdot \underline{\underline{\mu_{cz}}} \cdot \underline{\underline{\varepsilon_{cz}}} - (3 \lambda_{cz} + 2 \mu_{cz}) \cdot \underline{\underline{\varepsilon_{imp2}}}(t) \quad (19)$$

345 where

346 $\underline{\underline{\varepsilon_{imp2}}}$ is the imposed strain applied to the cracked zone of the surrounding concrete due to
 347 presence of ASR gel in the cracks;

348 the displacement is

$$\underline{\underline{u_{cz}}}(r) = \left(A_{cz} \cdot r + \frac{B_{cz}}{r^2} \right) \underline{\underline{e_r}} \quad (20)$$

349 The two supplementary unknown constants A_{cz} and B_{cz} can be determined from two
 350 supplementary boundary conditions: the continuity of radial displacements and radial stresses
 351 at the boundary between the cracked zone and the surrounding concrete. The mechanical
 352 equations can thus be solved in function of R_{cz} , ε_{imp1} and ε_{imp2} . Three last equations are needed
 353 to assess the three unknown values of R_{cz} , ε_{imp1} and ε_{imp2} . The tensile stress $\sigma_{\theta\theta}$ is equal to the
 354 concrete tensile strength f_t for the radius R_{cz} :

$$\sigma_{\theta\theta}^{SC}(R_{cz}) = f_t \quad (21)$$

355 The effect of the imposed deformations ε_{imp1} and ε_{imp2} in the aggregate and in the concrete
 356 filled by the gel can be compared to a pressure p_g in both the aggregate and the cracked zone
 357 (Figure 5). As the pressure p_g is an isotropic stress, in the cracked zone filled by the gel

$$\sigma_{rr}^{cz}(R_{cz}) = \sigma_{\theta\theta}^{cz}(R_{cz}) \quad (22)$$

358 The imposed strains applied to the aggregate and to the cracked zone are the relative increase
 359 in the volume due to the production of gel by ASR. However, as explained above, a part of
 360 the gel fills the porous volume surrounding the aggregate (determined by equation 3) and does
 361 not participate in the expansion. The imposed strain is then equal to the volume of gel V_g
 362 minus the connected porosity V_{por} filled by the gel compared to the volume of the aggregate.
 363 Thus, the last equation is given by chemical modeling:

$$\langle V_g - V_{por} \rangle^+ = \frac{4}{3} \pi R_a^3 \varepsilon_{imp1} + \frac{4}{3} \pi (R_{cz}^3 - R_a^3) \varepsilon_{imp2} \quad (23)$$

364 where $\langle X \rangle^+$ is equal to X if $X > 0$ or equal to 0 if $X \leq 0$.

365 The damage to the concrete is obtained by substituting the volume of gel determined by the
 366 chemical modeling (Eq. 3) in Eq 23. The expansion induced by ASR in each aggregate size
 367 fraction can thus be calculated. For the aggregate size fraction a :

$$\varepsilon_a = \frac{u_{rr}(R_{REV}^a)}{R_{REV}^a} \quad (24)$$

368 with R_{REV}^a the radius of the REV corresponding to the aggregate size fraction i .

369 If the concrete contains several aggregate size fractions, the resulting strain is assumed to be
 370 the sum of expansions induced by each fraction:

$$\varepsilon_{ASR} = \sum_a \varepsilon_a \quad (25)$$

371 The relationship between the damage and the expansion of one reactive aggregate obtained by
 372 this model has been plotted in Figure 6. It is interesting to compare these values to
 373 experimental data but only a few papers deal with the decrease of direct tensile strength with
 374 ASR expansion, and none with the decrease of the tensile modulus. Siemes and Visser
 375 measured a decrease greater than 85% in the direct tensile strength for expansions between
 376 0.05% and 0.1% [37]. For the same ASR expansions (between 0.05 and 0.1%), the damage
 377 calculated by the model is between 60 and 75%, which is slightly lower than the experimental
 378 values.

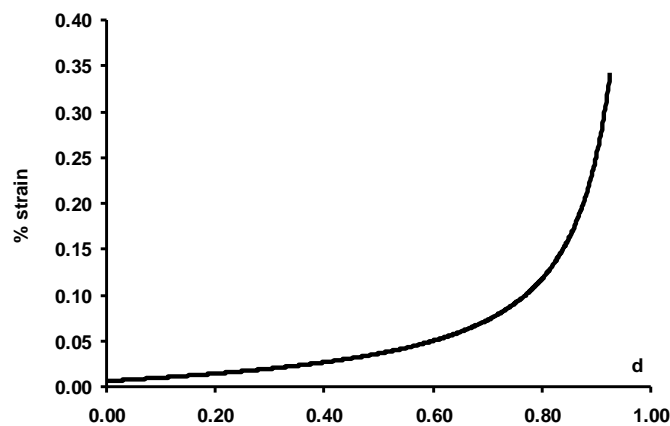


Figure 6 – Relationship between the damage (d) and the expansion of the REV

379

380 The mechanical modeling uses only five parameters: the Young's modulus and the Poisson's
 381 coefficient of the aggregate and mortar (E_a , ν_a and E_m , ν_m) and the tensile strength of the
 382 mortar f_t ; no other fitting is necessary.

383 **5. Comparison with experiments**

384 The last part of the paper shows some calculations performed with the model developed in the
385 previous parts. In order to assess the capability of the model to represent and predict real ASR
386 expansions, the analysis is divided into three parts. First, experiments used to fit and test the
387 model are presented. Then, the identification of the parameters is carried out and discussed.
388 For the identification, the measurements of expansion performed on four different mortars
389 were used. Finally, the model is used to calculate the expansion of six other mortars. The
390 calculated expansions are compared to the measured ones and the differences are discussed.

391 **5.1 Experiments**

392 The experiments used to check the capability of the model to predict ASR expansion have
393 been presented and analyzed in a previous paper [38]. Therefore, only the parameters used by
394 the model are dealt with here. Expansion was measured on mortar prisms with a water-cement
395 ratio of 0.5. The sand and cement contents were 1613.4 kg/m³ and 537.8 kg/m³ respectively.
396 Two distinct Na/Si ratios were studied by adjusting the alkali contents (Na₂O_{eq}) to 6.2 and
397 13.4 kg of alkali per m³ of mortar (addition of NaOH in the mixing water). Three size
398 fractions of aggregate were used: FS for small aggregates (80–160 μm), FM for medium
399 aggregates (315–630 μm) and FL for large ones (1.25–3.15 mm). The reactive aggregate was
400 a siliceous limestone. In the experimental study, only fractions FS and FL were composed of
401 reactive aggregates, the medium size aggregates were not reactive but were introduced into
402 the formulation to obtain an acceptable particle size distribution. The reactive silica contents
403 of the two reactive fractions were measured through a chemical analysis based on basic attack
404 [38]; the reactive SiO₂ contents were equal to 9.4% and 12.4% per kg of aggregate for FS and
405 FL. The particle size distribution was the same for all the mortars: 30% of FS, 40% of FM and
406 30% of FL. Different proportions of reactive and non-reactive aggregates from the two size

407 fractions FS and FL were used to make 5 reactive mortars for each alkali content, with always
 408 30% of reactive particles (Figure 7).

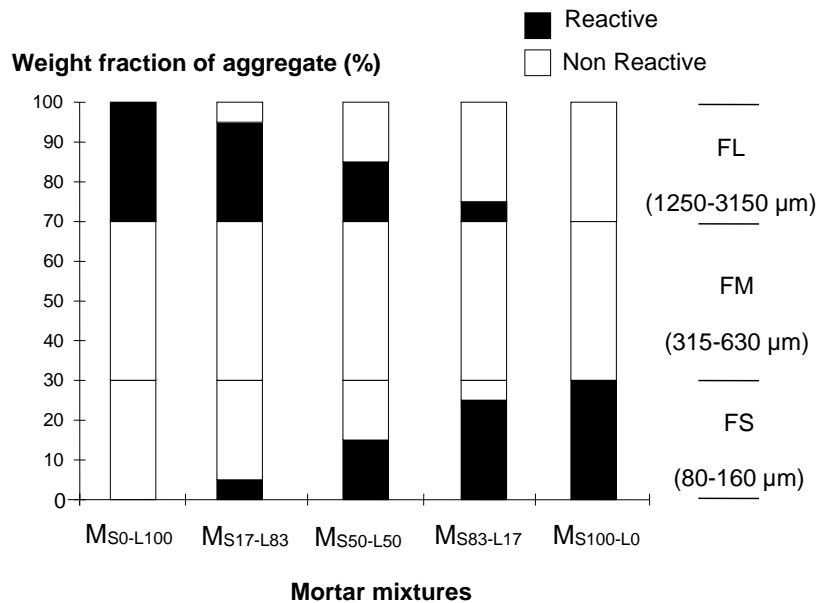


Figure 7 – Particle size distribution of the five mortars (in black: reactive aggregate, in white: non-reactive aggregate)

409
 410 The mortar $M_{S0-L100}$ contained 0% of reactive particles in the SL fraction while 100% of the
 411 particles of the FL fraction were reactive. For the mortar $M_{S100-L0}$, 100% of the smallest
 412 reactive particles (FS) were reactive and all the other particles were non-reactive. The reactive
 413 particle contents of the mortars $M_{S17-L83}$, $M_{S50-L50}$ and $M_{S83-L17}$, lay between these two values.
 414 The ASR expansions presented in Figures 8 and 9, and used for the identification of the
 415 parameters and for the analysis of the model were obtained by subtracting the expansion of
 416 the reference mortar (without reactive aggregate) from the total expansion [38]. Thus, the
 417 strains were only caused by the pressure of the ASR gel and not by the pressure due to water
 418 absorption. The water porosity of each of the mortars was measured at the end of the
 419 experiment (Table 1), using AFPC-AFREM method [39]. Values were between 17 and 20%.

Table 1 – Porosity of the mortars in %

Alkali content of the mix design	$M_{S0-L100}$	$M_{S17-L83}$	$M_{S50-L50}$	$M_{S83-L17}$	$M_{S100-L0}$
6.2 kg / m ³	17.5	16.9	17.3	17.6	17.6
13.4 kg / m ³	20	19.9	19.6	18.9	17.9

420 **5.2 Assessment of the parameters**

421 Table 2 sums up the various parameters of the two models, with the symbols, the method used
 422 for identification, the values and the units. The following parts explain how the values were
 423 obtained.

Table 2 – Parameter identification

Parameter	Symbol	Identification	Value	Units
Physicochemical modeling				
<i>Aggregate</i>				
Coefficient of diffusion	D	curve fitting	3.5×10^{-13}	m ² /s
Porosity	p	usual value	0.01	%
<i>Paste</i>				
Porosity of mortar	p_{mort}	measurement	17.-20.	%
Thickness of the connected porous interface zone	t_c	curve fitting	0.63×10^{-6}	m
<i>Gel</i>				
Molar volume of ASR gel	V_{gel}^{mol}	curve fitting	18.2×10^{-6}	m ³ /mol
Alkali threshold	N_{ath}	curve fitting	620.	mol/m ³
alkali fixation coefficient	f	curve fitting	$- 6.5 \times 10^{-7}$	m ³ /m ³ /s
Mechanical modeling				
<i>Aggregate</i>				
Young's modulus	E_a	usual value	70000.	MPa
Poisson's coefficient	ν_a	usual value	0.2	-
<i>Mortar</i>				
Young's modulus	E_{REV}	usual value	9000.	MPa
Poisson's coefficient	ν_{REV}	usual value	0.2	-
Tensile strength	f_t	usual value	3.	MPa

424

425 **5.2.1 Parameters of the physicochemical modeling**

426 The first parameters needed for the physicochemical modeling are given by the mix-design
 427 information (see above: size and volume fractions of particles, alkali and reactive silica
 428 contents). Taking all the information into account, the aggregate concentration per m³ of
 429 concrete C_{agg} could be calculated: it was equal to 0.61.

430 The porosity of the aggregate was taken as the value of 0.01% given by a previous work [40].

431 The porosity of the cement paste was calculated with equation 7. The last five parameters
 432 (coefficient of diffusion, thickness of the connected porous interface zone, molar volume of

433 ASR gel, threshold concentration Na_{th} and alkali fixation coefficient) of the physicochemical
434 modeling were obtained by curve fitting on four mortars of the experimental study as
435 explained in 5.2.3.

436 **5.2.2 Parameters of the mechanical modeling**

437 All the parameters of the mechanical modeling (Table 2) were obtained from the literature.
438 The Young's modulus of the siliceous limestone was determined in a previous experiment
439 [41]. The instantaneous Young's modulus of the mortar was taken as equal to a frequently
440 found value for a mortar with a ratio W/C of 0.5: about 27000 MPa. As explained in the
441 presentation of the assumptions, a long-term Young's modulus equal to one third of the
442 instantaneous Young's modulus was used in the calculations in order to take the creep effect
443 into account. The Poisson's coefficients of aggregate and mortar were taken as 0.2. The
444 tensile strength of the mortar was estimated at 3 MPa. None of the parameters of the
445 mechanical modeling were fitted.

446 **5.2.3 Identification by curve fitting**

447 The five parameters (coefficient of diffusion, thickness of the connected porous interface
448 zone, molar volume of ASR gel, threshold concentration Na_{th} and alkali fixation coefficient)
449 were obtained by curve fitting the expansions of four mortars of the experimental study: the
450 last expansion measured on $M_{S0-L100}$ with 6.2 kg/m^3 of alkali and M2, $M_{S100-L0}$ with
451 13.4 kg/m^3 of alkali, and the whole expansion curves of $M_{S50-L50}$ with 6.2 kg/m^3 of alkali and
452 $M_{S17-L83}$ with 13.4 kg/m^3 of alkali (Figure 8). First, the molar volume of ASR gel and the
453 thickness of the connected porous zone were determined to fit the last expansion measured on
454 the mortars $M_{S0-L100}$ - 6.2 kg/m^3 , $M_{S17-L83}$ and $M_{S100-L0}$ - 13.4 kg/m^3 (Figure 8). Then, the
455 coefficients of diffusion and fixation of alkali were calculated to fit the whole kinetics of the

456 expansion of the two mortars $M_{S50-L50}$ - 6.2 kg/m^3 and $M_{S17-L83}$ - 13.4 kg/m^3 (Figure 8). The
 457 values thus determined are given in Table 2.

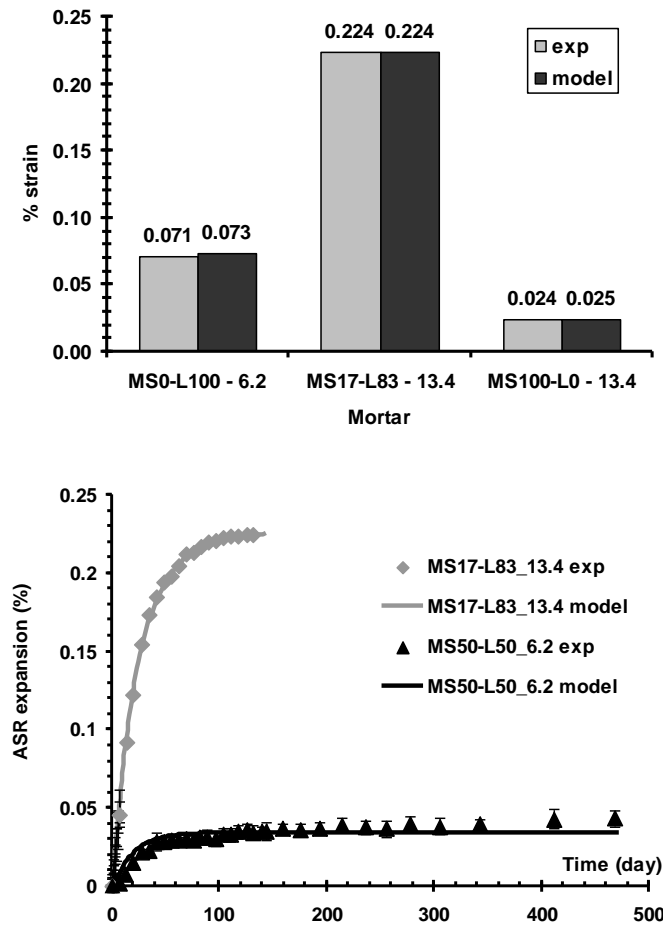


Figure 8 – Identification of chemical parameters on mortars $M_{S0-L100-6.2\text{kg/m}^3}$, $M_{S50-L50-6.2\text{kg/m}^3}$, $M_{S17-L83-13.4\text{kg/m}^3}$ and $M_{S100-L0-13.4\text{kg/m}^3}$

458

459 **5.3 Discussion**

460 **5.3.1 Curve fitting**

461 As shown in Figure 8, the determination of the five parameters of the physicochemical
 462 modeling allowed a good representation of ASR expansions to be obtained for two different
 463 reactive particle sizes and two different alkali contents. As already observed in the analysis of
 464 the experiment [38], the larger the aggregate, the higher the ASR-expansion. The model

465 explains the decrease of the expansion with the increase in the reactive particle sizes by the
466 movement of a part of the gel into the connected porous zone. The decrease of 90% observed
467 between the small fraction FS and the large fraction FL can be obtained by a thickness of the
468 connected porous zone of about $0.6 \mu\text{m}$. The second main parameter of the final expansions
469 of the mortars in the model is the molar volume of ASR gels. The molar volume determined
470 by curve fitting for this experiment, $18.2 \cdot 10^{-6} \text{ m}^3/\text{mol}$, is in good agreement with the
471 experimental values obtained on synthetic gels. In [42], the molar volume of synthetic gels
472 similar to natural ASR gels in solution was measured to be between $17.35 \cdot 10^{-6}$ and $23.65 \cdot 10^{-6}$
473 m^3/mol depending on the composition of the gels. The two last parameters have large effects
474 on the kinetics and on the expansion of mortar with low alkali content. Good representation of
475 the expansion curves was obtained with the values given in Table 2.

476 The threshold of alkali above which the ASR-expansion occurred was assessed by curve
477 fitting. With this threshold and all the parameters given in Table 2, for a mortar with a mean
478 porosity of 18%, ASR expansion occurs for alkali content higher than $4 \text{ kg of alkali /m}^3$ of
479 concrete. This is in good agreement with the usual values given by the literature (3 and
480 5 kg/m^3) [23-26].

481 **5.3.2 Prediction of other expansions**

482 Once the curve fitting had been performed, all the other expansions were calculated without
483 any additional fitting (Figure 9).

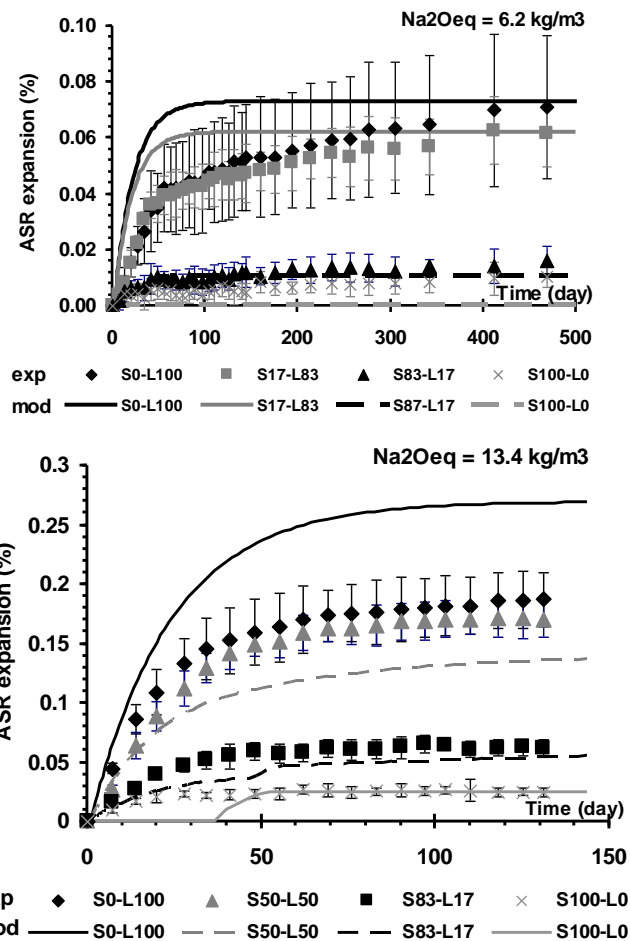


Figure 9 – Prediction of the ASR-expansion of the mortars $M_{S0-L100}$, $M_{S17-L83}$, $M_{S83-L17}$, $M_{S100-L0-6.2kg/m^3}$ and $M_{S0-L100}$, $M_{S50-L50}$, $M_{S83-L17}$, $M_{S100-L0-13.4kg/m^3}$

484

485 For the low alkali content, the kinetics appears to be overestimated but the final expansions

486 are well predicted. For the high alkali content, the mortars $M_{S50-L50}$ and $M_{S83-L17}$ are quite

487 well-estimated but the prediction of the mortar $M_{S0-L100}$ is not good. The differences between

488 the calculations and the measurements of the mortar $M_{S50-L50}$ can be explained by the

489 sensitivity of the model to the porosity of the cement paste. If the same porosity is taken for

490 the mortar $M_{S100-L0}$ used in the curve fitting and for the mortar $M_{S50-L50}$, the prediction is

491 perfect for the two mortars. A variation of 1.5% of porosity (it is the difference between the

492 two mortars of the high alkali content $M_{S50-L50}$ and $M_{S100-L0}$) gives a variation of about 0.03%

493 in the calculated expansions. The scatter (the porosity of $M_{S0-L100}$ lies between 19.5% and

494 20.7%) and the high value of porosity (about 20% for $M_{S0-L100}$, $M_{S17-L83}$ and $M_{S50-L50}$ with the

495 high alkali content) can be responsible for the difficulties experienced in obtaining better
496 agreement for the two mortars $M_{S0-L100}$ and $M_{S50-L50}$. The delay observed for the mortar M_{S100-}
497 $L0$ can be partly explained by the discretization of the particle sizes: in the present study only
498 one average size was used for each aggregate size range (S,M or L). A better description of
499 the size distribution of the finest particles could improve the modeling results.

500 **5.3.3 Interest and limitations of the model**

501 The model presented here is mainly based on a previous model developed by Poyet *et al.* [18].
502 Several improvements can be noted. In this new model, some considerations have been
503 modified:

- 504 - Due to the large difference in the diffusion coefficients of the aggregate and the
505 cement paste, the concentration of alkali in the paste has been considered as
506 homogeneous and is represented by a single variable (no more discretization of the
507 paste around each aggregate like in [18]). The calculated values remain reliable, but
508 the duration of calculation is largely reduced.
- 509 - In order to predict the difference of expansion, the mechanical part of the model
510 presents in [18] was partly based on a parameter which depends on the size of the
511 aggregates. Thus, it was not an intrinsic parameter of the material. In the new model,
512 all the mechanical parameters are intrinsic, i.e. independent of the aggregate size. The
513 expansions of aggregate of different size can be deduced without supplementary
514 fitting.
- 515 - The definition of a threshold in alkali concentration allows the expansions of mortars
516 containing different alkali contents to be calculated with a good accuracy. No previous
517 models in the literature were tested on this point.

518 Contrary to the previous model [18], the improved new model presented in this paper allows
519 the prediction of ASR expansions of mortars containing particles of different sizes.

520 However, the present model still has some limitations. One of the main difficulties in using
521 the model presented above is the determination of the reactive silica content in the aggregate.
522 A method was proposed in [38] for the siliceous limestone studied here, but improvements are
523 still required, particularly to be used for other types of reactive aggregates.

524 Some papers have shown the replacement of the alkali by calcium in the ASR gels [8-10].
525 This phenomenon has little effect on the expansion obtained in the laboratory for short
526 periods or for mortars with high alkali content because it appears to occur after long period of
527 exposure. However, it can have important effects on the final expansion in real structures
528 because, once free again, alkali can attack more reactive silica and new expansions are
529 possible [6-7]. Therefore, it will be the next improvement made to the model.

530 Moreover, the model was developed with several assumptions (about the diffusion, the
531 composition of the ASR gel, the mechanical properties of mortar under long-term loading,
532 etc.). Supplementary investigations are needed before it can be applied to real structures. In
533 particular, the effect of temperature on all the physiochemical and mechanical mechanisms
534 needs to be analyzed (expansion measurements of mortars kept at several temperatures are
535 currently in progress). This paper has shown the effect of the aggregate size on the prediction
536 of the concrete expansion. It should be taken into account in the expert assessments of real
537 structures already performed in [6-7]. Thus, it would be important to study the effects of the
538 discretization of the aggregate size distribution on the expansion predicted.

539

540 **6. Conclusion**

541 This paper presents an improved empirical microscopic model of ASR expansions based on
542 previous models. It proposes some improvements to take the fixation of alkali into account
543 and to calculate the ASR expansion by means of a mechanical damage variable. The diffusion
544 and the fixation of the alkali are assessed with the mass balance equation. A threshold alkali
545 concentration, above which the formation of the gel starts, is defined; the speed of alkali
546 fixation is assumed to be proportional to the difference between the alkali concentration in the
547 aggregate and this threshold. The mechanical modeling uses a damage variable in order to
548 determine the ASR expansion due to the volume of gel produced by the reaction and
549 determined by the physicochemical part of the model. No parameter of the mechanical model
550 needs fitting. Previous experimental research has been used to check the capability of the
551 model. Four parameters of the physicochemical modeling were determined by curve fitting
552 the expansion curves of four mortars of this experiment. These model parameters have a
553 physical meaning and have been found to be close to previous measurements reported in the
554 literature. The model can reproduce the decrease of expansion with the size of the aggregate,
555 and the increase of expansion with the alkali content. The model is also able to predict the
556 expansions of six other mortars containing two sizes of aggregate and cast with two alkali
557 contents. These calculations have shown the sensitivity of the model to the mortar porosity.
558 Finally, the academic interest of the model lies in the fact that the significance of every
559 assumed mechanism is explained and quantified.

560 Real structures containing large reactive aggregate (size about 100 mm) are currently being
561 analyzed in the LMDC by using the same assumptions as in this model. In this approach, the
562 largest aggregates are crushed and used to make new mortars with high alkali contents in
563 order to quantify the reactive silica remaining in affected concrete aggregate as rapidly as

564 possible [7]. Kinetics parameters are assessed on these mortars and the model is used to
565 predict the expansion of larger aggregates with different alkali contents. Thus, the model
566 could be used to predict the slow expansion of concrete in structures from the fast expansion
567 of mortar observed in the laboratory.

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669 **Acknowledgments**

670 The authors are grateful to Electricité De France for supporting this work.

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672 **Notations**

673 a sub or superscript relative to the size fraction of the reactive aggregate

674 C_{agg} volume fraction of all the aggregate per m^3 of concrete

675 C_{Na} concentration of alkali

676 C_{Na}^{cp} alkali concentration in the cement paste

677 CZ subscript relative to the cracked zone surrounding the reactive aggregate

678 D coefficient of diffusion of alkalis into the aggregate

679 d damaged variable

680 $\underline{\underline{\varepsilon}}$ strain matrix for each material

681 ε_a expansion induced by ASR in the aggregate a

682 ε_{ASR} total expansion of the concrete

683 ε_{imp1} imposed strain applied to the aggregate

684 ε_{imp2} imposed strain applied to the cracked zone

685 E Young's modulus

686 E_d damaged Young's modulus

687 ϕ_a volume fraction of reactive aggregates with mean radius R_a

688 f coefficient of fixation of alkali

689 f_t tensile strength of the mortar

690 $\underline{\underline{I}}$ unit matrix

691 M_{Na2O} mass of equivalent alkali per m^3 of concrete

692 M^{mol}_{Na2O} molar mass of equivalent alkali (equal to 0.062 kg/mol)

693	ν	Poisson's coefficient of the medium
694	N_a	number of reactive aggregate a in the final REV
695	Na_{th}	alkali threshold above which the attack of reactive silica starts
696	n_g^a	number of moles of ASR-gel produced by the aggregate a
697	p_{agg}	porosity of the aggregate
698	p_{cp}	porosity of the cement paste
699	p_{mort}	porosity of the mortar
700	R_a	mean radius of the reactive aggregate of size fraction a
701	R_{REV}^a	REV radius corresponding to the aggregate size fraction a
702	$\underline{\underline{\sigma}}$	stress matrix for each material
703	$S(C_{Na})$	depletion term which represents the alkali consumption
704	SC	subscript relative to the concrete surrounding the reactive aggregate
705	S_r	saturation degree
706	t_c	thickness of the connected porous volume filled by the gel
707	u	displacement
708	V_g	total volume of ASR gel produced
709	V_{gel}^{mol}	molar volume of the gel
710	V_{po}	volume of porosity filled by the gel
711	$\langle X \rangle^+$	equal to X if $X > 0$ or equal to 0 if $X \leq 0$
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