

Expansion modelling based on cracking induced by the formation of new phases in concrete

Stéphane Multon, Alain Sellier

▶ To cite this version:

Stéphane Multon, Alain Sellier. Expansion modelling based on cracking induced by the formation of new phases in concrete. International Journal of Solids and Structures, 2019, 160, pp.293-306. 10.1016/jijsolstr.2018.11.001 . hal-02056401

HAL Id: hal-02056401 https://hal.insa-toulouse.fr/hal-02056401

Submitted on 4 Mar 2019

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Expansion modelling based on cracking induced by the

formation of new phases in concrete

Stéphane Multon a* and Alain Sellier a

(a) Université de Toulouse; UPS, INSA; LMDC (Laboratoire Matériaux et Durabilité des Constructions); 135, avenue de Rangueil; F-31 077 Toulouse Cedex 04, France

Abstract

Unexpected expansion can be a cause of damage in quasi-brittle materials such as concrete, fired clays or rocks. Such expansions can be due to chemical reactions (alkalisilica reaction – ASR, sulfate attack) or physical phenomena (frost, transport of fluids). Expansion is caused by two main mechanisms: matrix deformation due to the pressure initiated by the formation of new phases in the porosity of the material, and matrix cracking, which increases the apparent swelling of the matrix. In this work, a poromechanical model is proposed to reproduce expansion in materials resulting from single or multiple pressures. In this model, plastic deformation is used to represent permanent strain due to diffuse cracking induced by the pressure. In the case of expansion in quasi-brittle materials, the permanent deformations induced by the pressure are anisotropic to take account of the impact of the initial material anisotropy and stress anisotropy on cracking. The model is then coupled with a damage model and used to evaluate the opening of localized cracks due to a pressure gradient in a laboratory specimen.

Keywords

27 Anisotropy, cracking, expansion, plasticity, pressure.

^{*} Corresponding author, *e-mail address*: multon@insa-toulouse.fr (Stéphane Multon)

1. Introduction

31 Damage due to expansion in materials decreases the service life of structures. 32 Unexpected expansion can be responsible for cracking in concrete, fired clays or other 33 quasi-brittle materials and mechanical modelling should be able to evaluate their 34 behaviour at material and structure scales. External or internal chemical attacks (Alkali-Silica Reaction – ASR [1], Delayed Ettringite Formation – DEF [2], external sulfate 35 36 attack [3], expansion of resins embedded in quasi-brittle materials [4]) or physical 37 phenomena (frost [5]) can be the cause of such swelling and lead to a decrease in the 38 strength of the materials affected. For quasi-brittle materials, irreversible deformation due 39 to cracking induced by pressure is the main cause of the positive strain of expansion. The 40 balance between local stresses around expansive new phases and stresses due to external 41 loading leads to anisotropic cracking. Given the dependence of the pressure on 42 environmental conditions, the development of such expansions can also lead to 43 deformation gradients both in real structures and in specimens studied under laboratory 44 conditions. The consequence is the opening of localized cracks on the skin of the 45 concrete. 46 Modelling should be able to distinguish and to assess the contribution of each 47 mechanism: pressure, diffuse cracking due to material damage, and localized cracking 48 due to pressure gradient. 49 In this work, a poromechanical model is proposed and used to quantify expansion in 50 concrete. First, the determination of the pressure according to the volume increase of new 51 phases in the material is described within the framework of poromechanics [6], [7]. In 52 particular, the case of alkali-silica reaction, for which pressure occurs in inclusions 53 (aggregate) embedded in the material (concrete) is addressed as a case for which up-54 scaling and multiple pressures should be considered. Plasticity is commonly used to 55 represent permanent strain of quasi-brittle materials [8], [9]. In the present work, plastic 56 deformation is adopted to model the permanent strain due to the diffuse cracking caused 57 by the pressure. The criteria associated with these deformations are orthotropic so as to

- 58 consider the impact of an anisotropic stress state on expansions [10], [11]. The model is
- 59 then used to reproduce the swelling anisotropy induced either by the anisotropic initial
- 60 strength of certain materials, or by the anisotropy due to the stress state. The analysis
- 61 highlights the importance of cracking in the mechanisms of expansion in concrete.

62 2. Pressure

- 63 Because of their low strength in tension, the elastic deformation of quasi-brittle materials
- 64 under internal pressure is small. Cracking thus plays an important role in deformations
- and has to be accurately determined. After cracking, the evolution of irreversible
- 66 deformation under the effect of expansive phases is still driven by their pressures.
- 67 Therefore, the same care has to be taken when evaluating pressure or anisotropic
- 68 permanent strains corresponding to the induced cracking.

69 2.1 Pressure due to the formation of new phases

- 70 The pressure induced by the formation of new phases in materials depends on the amount
- and the nature of the reactive components [12]–[21], on the structure of the material
- 72 porosity [22]-[25] and on the capability of the porous material to tolerate induced
- 73 tension. The interactions between the swelling inclusions and the matrix determine the
- 74 pressure developed in the swelling phase. In this work, the pressure, p_i , in the porous
- 75 material due to inclusion i is determined in the framework of poromechanics [6], [7]
- 76 through the following equation:

$$p_i = M_i \cdot (\varphi_i - \varphi_i^0 - \varphi_p - \varphi_{cr}) \tag{1}$$

- 77 with:
- 78 M_i the Biot Modulus related to the inclusions,
- 79 φ_i , the volumetric fraction of porosity filled by the inclusions related to the skeleton
- 80 deformation [23]. It can be assessed from the growth of the new phases in relation to
- 81 crystallization pressure [12], [13], [23] or to the volume produced by chemical reaction
- 82 [14], [26].
- 83 φ_i^0 is the volumetric fraction of new phases leading to little expansion during the reaction
- 84 for mechanical reasons (migration in porosity [25], [27]–[29], formation in pores too

- large to induce pressure [14], [22], [30]) or chemical reasons (composition of the phases
- 86 [31]–[33] or non-expansive surface absorption [34]). It is taken to be proportional to the
- 87 pressure:

$$\varphi_i^0 = \varphi_{ref} \cdot \frac{p_i}{p_{ref}} \tag{2}$$

- 88 φ_{ref} is a reference volume. It corresponds to the volume of new phases formed for the
- 89 pressure p_{ref} that leads to the first cracking at material scale in free swelling conditions.
- 90 It can be related to the pore distribution [14], [27] or be calibrated to obtain the delay at
- 91 the beginning of the expansion curve.
- 92 φ_p is the volumetric deformation due to elasticity of porosity filled by the inclusion
- 93 of new phases, and delayed deformation (diffuse cracking due to the pressure and
- structural cracks are not considered in this term but in φ_{cr} as explained below), which
- 95 can be calculated with b_i , the Biot coefficient related to the expansive inclusions:

$$\varphi_n = b_i \cdot (\varepsilon - \varepsilon_{cr} - \varepsilon_{an}) \tag{3}$$

- Here, ε is the mechanical deformation of the porous material, and ε_{cr} its deformation due
- 97 to cracking induced by the pressure. The impact of ε_{cr} on pressure is considered in (1)
- 98 with an interaction coefficient of 1, and thus greater than the Biot coefficient used in (3).
- 99 ε_{an} is the deformation due to structural cracks that are not connected to the sites of
- 100 formation of inclusions and so cannot have a direct impact on the pressure.
- In equation (1), φ_{cr} is the volume of diffuse cracks caused by the pressure; it is equal to
- 102 the volumetric deformation of the porous material due to the diffuse cracking ε_{cr} . In this
- equation, for the sake of simplicity, this volume is assumed to be totally filled by the new
- phases. The main assumption of the model is then that the new phases can migrate only
- toward the cracks they have themselves created.
- 106 The role of φ_{cr} in Equation (1) is particularly important for the modelling of such
- phenomena. If at least one direction is free of compressive stress in the material, the
- pressure p_i cannot increase very greatly as cracking is possible perpendicularly to the free
- 109 direction. This is taken into account through φ_{cr} . If φ_{cr} increases, the stabilization of the
- 110 pressure p_i can be obtained. This stabilization of the pressure is necessary to obtain

realistic stress in cases of restraint, as observed in experimentally [30], [35]–[38]. This

point is highlighted in the part that focuses on cracking.

113

114 M_i , the Biot Modulus related to the inclusions, depends on the volume of new phases φ_i

and on the mechanical properties of the matrix (bulk modulus K_m) and the inclusions [6],

116 [7], [24]. m is the subscript related to the matrix, including solid and porosity that is not

filled by the new phase inclusions. It is evaluated with the following equation:

$$\frac{1}{M_i} = \frac{b_i - \varphi_i}{K_m} + \frac{\varphi_i}{K_i} \tag{4}$$

118 If the new phases are taken to be spherical and embedded in a homogeneously solid

matrix [24]; b_i , the Biot coefficient related to the inclusion, can be estimated using a

120 Mori-Tanaka scheme for the estimation of the bulk modulus, K, of the porous material

121 [39]:

$$b_i = 1 - \frac{K}{K_m} = \frac{\varphi_i(3K_m + 4\mu_m)}{(3K_m\varphi_i + 4\mu_m)}$$
 (5)

122 with μ_m , the shear modulus of the matrix.

123 For simplicity, the Biot coefficient is evaluated in a linear context here, from the

mechanical properties and volumes of inclusions (Equation (5)) without consideration of

the shape of the porosity filled by the new phases. More precise quantification could be

obtained by taking account of the shape of filled cracks as proposed in [26], [27], [40]. In

the present work, the non-linearity due to the combination with diffuse cracking caused

by pressure, creep [41] and structural damage [42] is considered differently, by resorting

to damage theory [53].

130 The advancement of the new phases production can be evaluated with physicochemical

131 considerations or empirical laws. The aim of the paper is to focus on mechanical

132 considerations. As the chemical advancement is usually not impacted by mechanical

conditions in the case of the expansion due to new phases formation in concrete [43], the

134 chemical advancement can be separated of the mechanical problem. The equations

presented in this paper can thus be used whatever the approach applied to determine the

chemical advancement (theoretical or empirical approaches [12], [15], [17], [18], [20],

137 [21], [25], [44]).

The volumetric fraction of porosity filled by the inclusions can be considered as a data and its determination is summed up by the following equation:

$$\varphi_i(t) = n_i^{max} \cdot \varphi_i^{mol} \cdot A(t) \tag{6}$$

With n_i^{max} , the maximal number of moles of the new products which can be formed in the material, φ_i^{mol} , the molar volume of the new phases and A(t), the advancement of the reaction.

2.2 Case of porous materials embedded in another material

In some cases, the expansive inclusions can be formed in porous materials embedded in other materials. For example, Alkali-Silica Reaction (ASR) expansion can occur in aggregates embedded in concrete [45]–[48]. In this situation, scale-up is necessary to evaluate, firstly, the impact of the formation of new phases on the lower scale matrix (LS in Figure 1, for example the aggregate) and, secondly, the impact of the pressure of the lower scale matrix on the macro scale (MS in Figure 1, for example, the concrete). The volumetric fraction of the embedded material per volume of the macro scale material is referenced as φ_a . Moreover, the material embedded in the macro scale material can have different sizes and volumetric fractions and lead to multiple pressures [4], [27]. The pressure of each fraction p_a is different and should be evaluated separately.

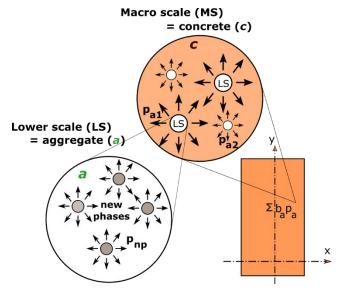


Figure 1: Porous material (Lower Scale, LS) embedded in another porous material (Macro Scale, MS)

154 The three equations of the multi-scale approach used to evaluate the pressure due to the

new phases p_{np} on the lower scale matrix (Equation (7)), the resulting pressure of the 155

lower scale p_a on the macro scale (Equation (8)) and finally the action of the multiple 156

pressures p_a of the lower scale matrix on the macro scale (Equation (9)) are: 157

$$\begin{cases} p_{np} = M_{np} \cdot \left(\varphi_{np} - \varphi_{np}^{0} - \varphi_{p} - \frac{\varphi_{cr}}{\varphi_{a}} \right) \downarrow \text{From new phases to lower scale} \\ p_{a} = b_{np} \cdot p_{np} & \downarrow \text{From lower scale to macro scale} \\ \tilde{\sigma}_{s} = K_{m} \cdot \left(\varepsilon - \varepsilon_{an} \right) - \sum_{a} b_{a} \cdot p_{a} \end{cases}$$

$$(7)$$

$$\begin{cases} p_a = b_{np} \cdot p_{np} & \text{\downarrow From lower scale to macro scale} \end{cases}$$
 (8)

$$(\tilde{\sigma}_s = K_m \cdot (\varepsilon - \varepsilon_{an}) - \sum_a b_a \cdot p_a \tag{9}$$

The interactions between the three equations and the different terms of the equations are 158

159 explained in the three following subparts:

160

161 Pressure of new phases (NP) on the lower scale (LS) material

- 162 At the lower scale, the inclusion i (i = np at this scale) is the new phases, and the matrix,
- 163 m (m = a at this scale) is the lower scale (LS) matrix. As the expansive inclusions are
- 164 formed at the lower scale (Figure 1), the pressure induced by the formation of new phases
- 165 on the LS matrix can be defined from Equation (7).
- φ_{np} , φ_{np}^0 and φ_p are defined above and have to be determined per unit of volume of the 166
- lower scale matrix (here the aggregate). M_{np} and b_{np} related to the new phases are 167
- 168 evaluated from Equations (4) and (5).
- 169 As the cracks induced by the pressure of the new phases are usually connected with the
- 170 cracks at macro scale [48], the volume of cracks φ_{cr} in which the new phases can migrate
- 171 is taken to be the crack volume available in the macro scale material. At the scale of the
- 172 aggregate, this volume has to be normalized according to the volumetric fraction of
- aggregate φ_a in order to be obtained per unit of volume. Consequently, the impact of the 173
- 174 crack volume on pressure is fully considered at this lower scale.

- 176 Pressure of the lower scale (LS) material on the macro scale (MS) material
- 177 At the macro scale (Figure 1), the inclusion i (i = a at this scale) is the aggregate, and the
- 178 matrix m (m = c at this scale) is the concrete. M_a and b_a , related to the aggregate, are
- 179 evaluated from Equations (4) and (5).

180 The material at macro scale subjected to the pressure of the aggregate is under tension.

181 Because of its low tensile strength, the impact of its rigidity on aggregate pressure is

182 negligible compared to the impact of the crack volume, which was considered at the

lower scale. The pressure induced by the lower scale (aggregate) on the macro scale

184 (concrete) can thus be evaluated from Equation (8).

185

186 Consequence on pressure at the macro scale (MS) in case of expansive inclusions having

187 different sizes

As proposed in [7], [24], [26], the impact of multiple pressures on the macro scale

material can be obtained by summing the pressure, taking Biot coefficients into account.

190 The constitutive equation for the mean stress $\tilde{\sigma}_s$ at macroscopic scale is then Equation

191 (9).

In this case of multiple pressures, the volume of cracks of the macro scale material (φ_{cr}

in equation (7)) has to be distributed among the different fractions of aggregates (φ_a). In

this work, the distribution is assumed to be proportional to the volume of the new phases

195 φ_{np} a leading to cracking (so the volume of phases higher than φ_{np}^0 in equation (10)). For

material containing several sizes, a, of aggregate, it is necessary to distinguish the new

197 phases created by each aggregate: φ_{np_a} is the volumetric fraction of new phases created

198 in aggregate a and $\varphi^0_{np_a}$ is the volumetric fraction of new phases necessary to start

199 cracking in aggregate a. Thus, the volume of the crack induced by aggregate a is

200 evaluated by (10):

$$\varphi_{cr}^{a} = \frac{\langle \varphi_{np_a} - \varphi_{np_a}^{0} \rangle^{+}}{\sum_{a} \langle \varphi_{np_a} - \varphi_{np_a}^{0} \rangle^{+}} \varphi_{cr}$$
(10)

201

202 For expansion in quasi-brittle materials, the model considers damage through a coupling

with the modelling presented in [42]: the coupling method consists of affecting $\tilde{\sigma}_s$ by the

204 damage according to the principle already presented in [11] (Equation (11)):

$$\sigma_{S} = \tilde{\sigma}_{S} \ (1 - D) \tag{11}$$

The damage variable, D, depends on the permanent strain related to the diffuse cracking

and on the effective stress $\tilde{\sigma}_s$ due to the external loading.

207 Creep of the matrix, simultaneous with expansion, is also considered so as to obtain a 208 realistic evaluation of concrete damage at micro and macro scales [11], [49]: ε_{an} is the inelastic strain due to creep and cracking at the macro-scale. Creep is considered through 209 210 the model presented in [41] combined with the damage model proposed in [42] according 211 to the combination method described in [11].

3. Cracking

212

213

215

221

225

227

3.1 Diffuse cracking due to pressure

214 In stress free conditions, the diffuse cracking induced by the pressure can be isotropic (sulfate attack [38]) or anisotropic (alkali-silica reaction [50], [51], and frost in fired clays 216 [52]). In the absence of external loading, anisotropic expansion can be explained by the 217 initial anisotropy of the materials, for instance by the shape and the orientation of the 218 expansive inclusion (Figure 2). At the scale of the porous material, the mean stress field 219 is homogeneous. For uniformly distributed spherical inclusions, no direction is 220 preferential in stress free conditions (Figure 2). In this case, the cracking direction should be isotropic at the representative volume scale. For flattened inclusions oriented in a 222 preferential direction, the stress induced by the pressure at the points with the smallest 223 radius is larger than anywhere else (Figure 2). This leads to anisotropic cracking. The 224 presence of water pockets under the expansive inclusions can also cause orientation of cracking [53]. In the absence of loading, this effect can be evaluated through the following anisotropic cracking criteria f_i according to f_t , the tensile strength of the 226 porous material:

$$\begin{cases}
f_I = k_I \cdot p_{np} - f_t \\
f_{II} = k_{II} \cdot p_{np} - f_t \\
f_{III} = k_{III} \cdot p_{np} - f_t
\end{cases}$$
(12)

 k_i are the stress concentration factors in the three main directions of the aggregate shape 228 and p_{np} the pressure of the new phases produced in the embedded materials and 229 responsible for the diffuse cracking. 230

If one of these criteria f_i becomes higher than zero, cracks appear along this direction. In 231 232 the absence of loading, the cracks appear first in the plane perpendicular to the direction 233 having the largest stress concentration factor.

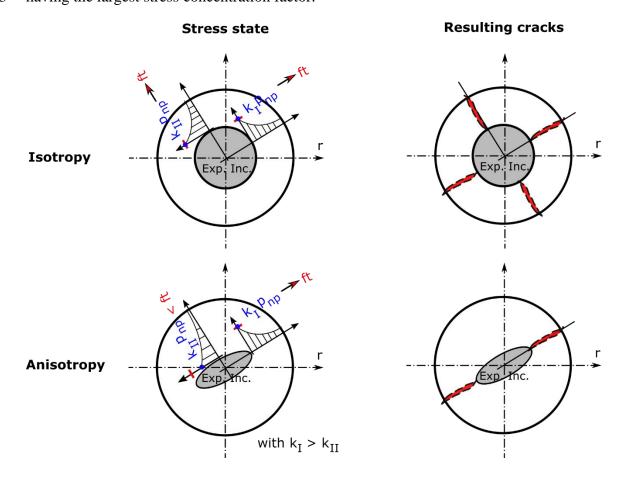


Figure 2: Ortho-radial stress state around spherical and penny-shaped inclusions from continuous mechanics and resulting cracks

With the simplified assumption of spherical inclusions, k_I is independent of the 234 235 orientation and can be evaluated in a linear context from the proportion of new phases:

$$k_{I} = k_{II} = k_{III} = \frac{1 + 2 \cdot \varphi_{np_a}}{2 \cdot (1 - \varphi_{np_a})}$$
(13)

236 If the material is damaged by multiple pressures, the single stress used in the plastic criterion at the macro-scale has to consider all the crack initiation possibilities at smaller scales. For this purpose, the local stress is evaluated in proportion to the pressures

237

- 239 weighted by the volume of new phases φ_{np_a} leading to cracking (so the volume of
- 240 phases higher than φ_{np}^0).
- 241 According to the geometry of the inclusion, the stress concentration factor can be
- 242 dependent on the direction (Figure 2). For orthotropic inclusions, the ratio between the
- 243 stress concentration factors in the three main directions (I, II, III) of a penny shaped
- inclusion *a* (Figure 2) is defined by equation (14):

$$k_{II} = k_{III} = \rho_{ani} \cdot k_I \tag{14}$$

- 245 ρ_{ani} is the rate of anisotropy (less than 1).
- 246 If ρ_{ani} is equal to 1, the cracking in stress-free conditions remains isotropic in the
- 247 absence of external loading. If ρ_{ani} is less than 1, the cracking in stress-free conditions
- 248 becomes orthotropic and occurs first in the plane perpendicular to the direction I
- 249 (Equation (14), Figure 2). This leads to anisotropic expansions.

250 3.2 Anisotropy of cracking due to macroscopic stress state

- 251 Under anisotropic mechanical loading, expansions are anisotropic [36], [37], [43], [54]–
- 252 [57]. For different natures of new phases (alkali silica gels or ettringite), a difference of
- 253 1 MPa in stress compared to the mean stress in the material is sufficient to cause
- 254 anisotropic expansion [36], [38], [54], [58].
- 255 Expansion anisotropy in materials subjected to loading is due to anisotropy of cracking. It
- 256 can be explained by the balance between the stresses induced by expansion around the
- 257 inclusion and the stresses due to external conditions. In stress free conditions, the
- 258 material is subjected to tensile stress around the expansive inclusions and the resulting
- 259 crack distribution is theoretically isotropic if the inclusions are isotropic and uniformly
- 260 distributed (Figure 3). Under compressive stresses, the tensile stresses are reduced (or
- even cancelled by the compressive stresses due to the external loading) in the direction
- 262 parallel to the compressive stress and cracking is prevented in the direction perpendicular
- 263 to the applied load (Figure 3). The stress state is not modified along the direction
- perpendicular to loading and cracking appears when, locally, the stress reaches the tensile
- strength (Figure 3). This explains why the cracks are usually parallel to the compressed
- 266 direction or to the restraint whatever the nature of the new phases [30], [35], [38], [43].

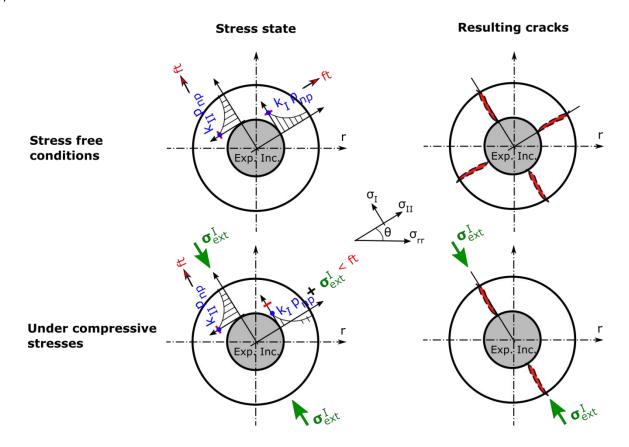


Figure 3: Idealized stress state around expansive inclusion, and resulting cracks. Due to the stress field shift towards compression, the failure criterion cannot be reached perpendicular to the applied compression, but only parallel to it

Once cracks occur in one direction, the following expansions change since the new phases can flow into or be formed in the cracks and pressure can be preferentially exerted perpendicular to the cracks. In cases of compression along two directions, cracking can occur parallel to the loading plane. In presence of loading, the anisotropic diffuse cracking can be evaluated through the following criteria f_i :

$$\begin{cases}
f_{I} = k_{I} \cdot p_{np} + \tilde{\sigma}_{I} - f_{t} \\
f_{II} = k_{II} \cdot p_{np} + \tilde{\sigma}_{II} - f_{t} \\
f_{III} = k_{III} \cdot p_{np} + \tilde{\sigma}_{III} - f_{t}
\end{cases}$$
(15)

with $\tilde{\sigma}_I$ the external stress in the material without damage (effective stress) in the main direction I of stresses (in this case, the stress concentration factors k_I are computed in the main direction of stresses).

- For cracking to occur in stress-free conditions, the local tensile stress, equal to $k_I \cdot p_{np}$,
- 277 has to be greater than the local strength f_t (Equation (12)). In cases of compressive stress
- 278 induced by external loading, $\tilde{\sigma}_I$ is negative (Equation (15)). To lead to cracking, the local
- 279 stress induced by the pressure $(k_I \cdot p_{np})$ has to be higher than the sum of the tensile
- 280 strength and the absolute value of the compressive stress.
- As the loading stress $\tilde{\sigma}_I$ is limited by the tensile strength f_t in the direction I [42], the
- 282 diffuse cracking depends directly on the pressure of the new phases for a material cracked
- 283 by external loading. The criterion becomes:

$$f_I = k_I \cdot p_{np} \tag{16}$$

- 284 If the external principal stresses do not coincide with the material main directions, the
- 285 stress concentration factors are determined in the principal directions of stresses
- according to elliptic approximations. Thus, the cracks orientation is mainly driven by the
- 287 external principal stresses which is usually observed in real cases.

3.3 Pressure evolution during diffuse cracking

- 289 The volume of new phases changes over time: frost can disappear with increasing
- 290 temperature, alkali-silica gels can lose water when exposed to dry conditions, etc. After
- such modifications, a large part of the expansion remains unchanged [5], [50], [59], so
- 292 the diffuse cracking induced by expansive phenomena does not appear to be reclosed.
- 293 This can be explained by the relative displacements of the lips of rough cracks. Lip
- 294 displacements lead to irreversible strains. This situation is modelled by means of the
- 295 plasticity theory that has already been used to represent permanent strain in quasi-brittle
- 296 materials [8], [9]. A plastic criterion is thus used to manage the permanent strain due to
- 297 the diffuse cracking induced by the pressure. It has already been used to model ettringite
- 298 formation [60] and alkali-silica reaction [61] expansions subjected to stress at macro-
- scale. In these previous works, the anisotropy of cracking with loading (Figure 3) was
- 300 already considered but, in the present paper, the plastic criterion is modified to also
- 301 consider a possible initial anisotropy of the material through the inclusion shape.

The behaviour of quasi-brittle materials subjected to expansion after first cracking has to be linked to experimental observations performed on specimens under restraint or applied stresses:

- Under restraint, the expansive mechanism leads to compressive stresses at macroscopic scale [30], [35]–[38]. In three experimental studies [30], [35], [36], rigid steel frames were used to strongly restrained expansion in one direction (the rigidity of the frames were largely upper than the rigidity of concrete specimens). In these three cases, for concrete expansion due to ASR or ettringite formation, the free swelling ranges from 0.1% to 8% and the resulting macroscopic uniaxial stress due to restraint lies between only 1 and 8 MPa [30], [35], [36] (Figure 4). The relation between free swelling and restraining stress appears to be quite linear between 0 and about 0.4%, with an increase of 1 MPa per 0.1% of free expansion. After 4 MPa, the increase of uniaxial stress with the free expansion slows down. In comparison, for a material with a Young's modulus of 30,000 MPa, an expansion of only 0.1% imposed on a perfectly elastic material would lead to restraint stress of 30 MPa.
- Under applied loading, the application of uniaxial compressive stresses of about 5 MPa is usually sufficient to stop expansion of about 0.2% in the loaded direction [43], [55]. Beyond this stress, the creep strains in the loaded direction appear to be the same as for creep in the material without expansion [43], [54], [55].

In these experiments, restraint and applied loading were uniaxial, and cracks could propagate in plans perpendicular to free directions. The new phases can fill this cracking, which delays the increase of the pressure in the porous materials and thus the resulting stress. As a result, the restraint stress is not so high as evaluated with the elastic assumption.

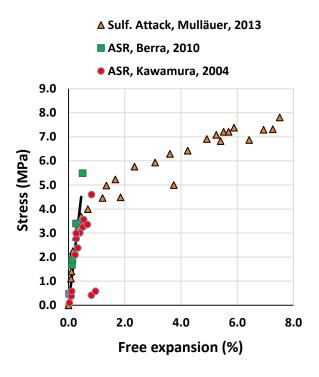


Figure 4: Restraint stress according to expansion in stress free condition for ASR-gels and ettringite in different strong restraint conditions [30], [35], [36].

This behaviour is taken into account through the combination of the pressure equation (Equation (1)) with the following hardening law (17). First, when cracking occurs, the volume of diffuse cracks φ_{cr} increases. The pressure p_i (Equation (1)) and the resulting macroscopic stress cannot increase too much. However, the first crack occurs in the weakest zone of the matrix. The tensile strength of the material after the first cracking increases continuously. The cracking process can continue only if the pressure grows in the zone that is not yet damaged. The stress has to increase in the undamaged zone (as observed in Figure 4) despite the fact that the specimen is free to swell in two directions (and restrained only in one direction). In this aim, a hardening law is proposed. This law has to be anisotropic as explained above:

$$\begin{cases}
R_{tI} = f_t + H \cdot \varepsilon_{pl}^{I} \\
R_{tII} = f_t + H \cdot \varepsilon_{pl}^{II} \\
R_{tIII} = f_t + H \cdot \varepsilon_{pl}^{III}
\end{cases}$$
(17)

338 with ε_{pl}^{I} , the plastic deformation in the main direction I. It represents the diffuse crack

339 opening in this direction. The sum of the plastic deformations in the three directions is

equal to φ_{cr} , the volume of diffuse cracks due to the pressure:

$$\varphi_{cr} = \varepsilon_{pl}^{I} + \varepsilon_{pl}^{II} + \varepsilon_{pl}^{III} \tag{18}$$

341 and

$$H = h_{crk} \cdot E \tag{19}$$

- 342 with h_{crk} the relative slope of the hardening law after cracking and E the elastic modulus
- of the macro scale material before cracking.
- 344 Accurate evaluation of stress level for restraint expansions is obtained by the combination
- of this hardening law with damage (Equation (11)) and creep modelling. The steeper the
- 346 slope of the hardening law after cracking, the higher the restraint stress obtained for a
- 347 given expansion. Figure 4 shows that the hardening law can be approximated by a linear
- 348 law for expansion lower than about 0.4%. The law should be nonlinear for higher
- 349 expansion (or at least bi-linear for the domain after cracking to consider the stiffness
- decrease of the matrix). In this paper, h_{crk} is equal to 0.025 except when this parameter is
- 351 the object of a parametric study.
- 352 For triaxial compressive applied loading, pressures first have to counteract the
- 353 compressive stress before inducing tension and have to be still greater to cause cracks.
- 354 For such multiaxial loading, the experiments in the literature show that the measured
- volumetric expansion decreases [56], [57]. In the model, as long as the cracking criterion
- 356 (Equation (15)) is not reached, the volume of cracking, φ_{cr} , stays equal to zero and the
- 357 pressure p_i increases (Equation (1)). As the pressure increases, φ_i^0 , the volumetric
- 358 fraction of new phases leading to small expansion also increases (Equation (2)) to
- 359 reproduce the dependence on pressure of the migration of phases in connected porosity
- 360 [56]. Thus, the pressure can never be too high even for triaxial compressive applied
- loading [61] and the resulting volumetric expansion decreases.
- 362 The implementation of this model is based, first, on a classical implicit return mapping
- algorithm [62] to solve the elasto-plastic problem, then the damage model [42] is applied

to the stresses deduced from the poro-plastic solution. The return mapping algorithm and the damage models are implemented in a non-linear finite element code. The method consists of first computing the evolution of the chemical reaction [63] versus the time step. Then, assuming visco-elastic behaviour of the poro-mechanical media, pressure and stress increments are computed according to the increment of strain. Once these increments have been added to the values of the last time step, the plastic criteria (15) are tested. If the criteria are exceeded, plastic flow is activated to return to the yield functions through the return mapping implicit method and the admissible stress state and pressure state obtained are used in the damage model to assess the apparent stress state. The finite element algorithm then computes the balance between the external forces applied to the structure and the internal forces corresponding to the stresses. If a force balance is not reached, the algorithm corrects the displacement field until equilibrium is reached.

4. Applications

The aim of this part is to evaluate the capability of the model to reproduce expansions in concrete in several situations. The validation is performed on concrete subjected to expansion due to alkali-silica reaction drawn from [50], [54]. In this study, the expansion occurred in reactive silica embedded in non-reactive limestone for two sizes of aggregates (Table 1). Thus, upscaling and calculations based on several pressures were used. The Young's moduli of the new phases, aggregate and concrete were taken to be 7 GPa [64], [65], 60 GPa [43] and 37.3 GPa [50] respectively. The moduli of the different phases used in the calculations are given in Table 2. The concrete tensile and compressive strengths were 4 and 38.4 MPa [50]. The behaviour of concrete in creep is available in [54].

In this application, the advancement was evaluated through mass balance equations solved for each size of aggregates, taking account of alkali diffusion (Equation (20)) and reactive mechanisms deduced from alkali fixation by ASR-gels (Equation (21)) [63]:

$$\begin{cases} p_{agg}S_r \frac{\partial [Na^+]}{\partial t} = div \left(D_a \overline{grad}[Na^+] \right) - \frac{\partial Na_f}{\partial t} \\ \frac{\partial Na_f}{\partial t} = \frac{\langle [Na^+] - [Na^+]_{(Ca,T)}^{thr} \rangle^+}{\tau_{ASR}} \end{cases}$$
(20)

with p_{agg} the aggregate porosity, S_r the degree of water saturation, $[Na^+]$ the alkali concentration in solution, Na_f , the amount of alkali bound in ASR-gels, D_a , the coefficient of diffusion of alkali in the aggregate, τ_{ASR} , the characteristic time of silica attack and $[Na^+]_{(Ca,T)}^{thr}$ the alkali concentration threshold below which the reaction products cause negligible expansion. This threshold depends on temperature T and calcium concentration, $[Ca^{2+}]$. In first approach, empirical relations can be used:

$$\begin{cases} [Na^{+}]_{(Ca,T)}^{thr} = 1540 \cdot exp \left[-\frac{205900}{R} \cdot \left(\frac{1}{T} - \frac{1}{T_{0}} \right) \right] \cdot [Ca^{2+}] \\ [Ca^{2+}] = 0.357 \cdot exp(386.8 \cdot [Na^{+}] - 0.01 \cdot T - 1.36 \cdot [Na^{+}] \cdot T) \end{cases}$$
(22)

396 With T in Kelvin and T_0 , equal to 293 K.

405

406

407

408

409

410

Usually, the molar ratio between silica (SiO₂) and alkali (Na₂O) present in ASR-gels in laboratory conditions is about 5 [64], [66]. The advancement of ASR-gel moles produced by one size of aggregate is then equal to the number of moles of silica attacked by alkalis divided by the maximal number of moles of the new products which can be formed in the aggregate:

$$A_a(t) = \frac{\frac{5}{2} \frac{\partial Na_f}{\partial t}}{n_i^{max}} \tag{24}$$

The fraction of new phases created before cracking, φ_{ref}^a , per volume of aggregate a (Equation (2)) was evaluated from the surface area of the aggregates. In this work, it was taken to be:

$$\varphi_{ref}^{a} = 1 - \frac{\left(R_{a} - d_{ref}\right)^{3}}{R_{a}^{3}} \tag{25}$$

with R_a the mean radius of the aggregate a and d_{ref} the distance used to evaluate the volume of new phases created before diffuse cracking. In reality, the volume of new phases formed before cracking is partly included in the aggregate porosity. For the sake of simplicity, only an average distance, d_{ref} , around the aggregate is considered. It is assumed not to depend on the aggregate size. The reference pressure (Equation (2)) is the pressure leading to the first diffuse cracking. p_{ref} depends on the tensile strength of the

porous material, f_t , and on aggregate shape through the stress concentration factor k_I (Figure 2):

$$p_{ref} = \frac{f_t}{k_I} \tag{26}$$

Table 1: Distribution of the aggregate embedded in the concrete studied [50], [54]

Aggregate reference (a)	Aggregate size (mm)	φ_a	b_a
1	4-12	0.10	0.19
2	12-20	0.32	0.49

Table 2: Mechanical properties of the different phases

Properties	New phases	Aggregate	Concrete
Young's modulus (GPa)	7	60	37.3
Poisson's ratio	0.2	0.2	0.2
Bulk modulus <i>K</i> (GPa)	3.9	33.3	20.7
Shear modulus μ (GPa)	2.9	25	15.5

4.1 Anisotropy in stress-free conditions

The model is first used to reproduce the anisotropic expansion due to a natural defect of the materials (Figure 2). In concrete, water pockets can form under aggregate particles, leading to stress concentrations (Figure 2) and thus to anisotropy [43], [53]. For the aggregate used in these experimentations, expansion was anisotropic in stress-free conditions: twice as large in the vertical direction as in the horizontal ones (circles in Figure 5). Isotropic expansion (calculated as the average expansion in the three directions

- to obtain the same volumetric expansion triangles in Figure 5) was first modelled with the following parameters:
- the coefficient of diffusion of alkali in aggregate, D_a : 5.e⁻¹⁴ m²/s,
- 426 the characteristic time of silica attack, τ_{ASR} : 400 days,
- 427 the molar volume of new phases, φ_{np}^{mol} : 15.5 cm³/mol,

445

446

447

448

449

450

- the average distance used to represent the volume of new phases created before diffuse cracking, d_{ref} : 5 μm.
- 430 The four parameters have been calibrated on the experimental data to reproduce the 431 isotropic expansions (Figure 5). They can be compared to experimental data of the 432 literature. The coefficient of diffusion of alkali in aggregate is smaller than the 433 coefficients measured in [67]. But such measurements are scarce, and the technique used 434 in this experimental work can be not totally representative of mechanisms occurring 435 during ASR-attack. The characteristic time of attack is slightly larger than the time 436 determined in [68] for opal, which can be expected due to the difference of silica nature 437 (opal is more reactive than aggregate used in this application). Molar volume of synthetic 438 gels similar to natural ASR gels in solution was measured to be between 17 and 24 439 cm³/mol depending on the composition of the gels [69]. The calibration is thus in good agreement with these experimental values obtained on synthetic gels. As d_{ref} is an 440 441 average distance, it cannot be directly compared to microscopic observations. However, it 442 can be supposed to be realistic as it is lower than usual interfacial transition zone between 443 aggregate and cement paste which can reach 20 µm [70], [71].
 - φ_{np_a} , the volume of new phases of the aggregate a at the time step t (Equation (7)), is proportional to the molar volume of new phases φ_{np}^{mol} according to the advancement of the reaction (Equation (6)). In this calculation, it leads to final volumes of gel φ_{np_1} and φ_{np_2} respectively equal to 1.9e-2 and 0.9e-2 m³ of new phases per m³ of aggregate (Table 3). As the kinetics is partly driven by ionic diffusion in spherical particles, the volume of new phases is the largest in the smallest reactive aggregate. The Biot coefficients and moduli computed for the new phases are given in Table 3. The Biot coefficient of the new phases in the smallest aggregate is larger than that in the largest

aggregate because of differences of volume of the phases. In this experiment, not all the reactive silica was consumed at the end of expansion. If all the silica had been consumed in all the aggregates, the same volume of new phases would have been created per volume of aggregate and thus the Biot coefficients would have been equal for the two aggregates.

The rate of anisotropy, ρ_{ani} , is then calibrated (and taken equal to 0.83) to obtain the anisotropic expansion (Figure 5). The criterion proposed in Equations (15) and (16) used with Equation (14) to obtain anisotropic cracking is then effective to reproduce the anisotropy of expansion in stress-free conditions with the same parameters (φ_{np}^{mol} and d_{ref}) as the averaged isotropic expansion. The formulation of the plasticity law for materials with high anisotropy of expansion in stress-conditions is thus validated. This feature of the model should be also supported by the comparison with expansion of the same material submitted to other stress levels. But experimental data with high anisotropic expansion are scarce and no experimental program have supplied data under various stress state for such materials.

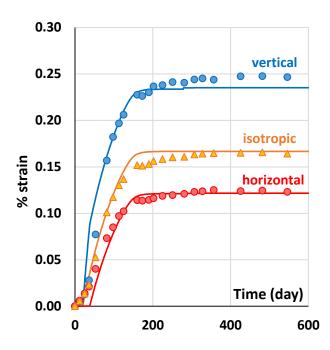


Figure 5: Isotropic or anisotropic stress-free expansion (circles: experimental points [50], triangles: averaged isotropic expansion deduced from experimental points, lines: modelling)

Table 3: Final volume of new phases and Biot coefficient and modulus for each aggregate class

Aggregate size	mm	4-12	12-20
$\overline{arphi_{np_a}}$	-	1.9e-2	0.9e-2
b_{np}	-	3.8e-2	1.8e-2
M_{np}	GPa	199.	429.

468

469

470

471

472

473

474

475

476

477

478

479

480

481

482

483

484

485

486

487

488

4.2 Expansion under restraint

The dependence of expansion on stress has to be well reproduced in order to obtain relevant modelling of real cases in specimens subjected to gradients or in real structures subjected to external loading or restraint due to boundary conditions. In the macro modelling proposed in [11], [61], which is efficient to reproduce structural behaviour, the Biot modulus and coefficient were used as calibration parameters to reproduce the behaviour of concrete subject to expansion and under mechanical loading and restraint. In the present work, the Biot modulus and coefficient are determined from the volume of new phases and from the mechanical properties of concrete, aggregate and new phases. In this case, only the slope of the hardening law after cracking h_{crk} in equation (18) is unknown. This parameter allows the pressure growth to be determined during the cracking process needed to explain the longitudinal stress increase observed in the experiments reported in Figure 4. The present paper proposes a parametric study to verify the capability of the model to reproduce the dependence of expansion on stress with only the slope of the hardening law as calibration parameter. The impact of h_{crk} on restrained stress is studied first. Three sets of parameters (Table 4) are determined for three significantly different values to obtain the same stress-free expansion (about 0.17% of isotropic linear expansion in Figure 5). The greater the slope of the hardening law, h_{crk} , the greater the pressure increase and the axial stress after cracking. In consequence, the molar volume φ_{nn}^{mol} necessary to obtain the same stressfree expansion has be to larger for a greater h_{crk} . This is due to the fact that, when

pressure growth is possible (when h_{crk} is great enough), the amount of gel migrating to the connected porosity also increases (see Equation (2)), so the amount of gel remaining in the inclusion to maintain the pressure would be smaller if the molar volume was not increased artificially to retrieve the correct free swelling.

Table 4: Modelling parameters for the study of restraint stress

h_{crk}	$arphi_{np}^{mol}$	d_{ref}
-	(cm ³ /mol)	(µm)
0.002	14.	4.5
0.025	15.5	5.
0.2	27.5	6.

Expansion under uniaxial restraint is then modelled. In this aim, the strain has been set to zero in the restraint direction. The numerical restraint stresses are plotted in Figure 6 for the three values of slope: the greater the slope, the larger the restraint stress. For h_{crk} equal to 0.002, the restraint stress is close to zero. This means that the pressure remains almost constant during crack propagation, as can happen for very fluid new phases (Figure 4 and Figure 7). In most cases, the restraint stress is about 1 MPa for 0.1% expansion and up to 0.4 or 0.5% expansion (Figure 7). A correct mean representation is obtained for a slope of about 0.025 (restraint stress of about 1.65 MPa for a final isotropic expansion of about 0.17%, Figure 7). For h_{crk} equal to 0.2, the calculation is closer to the elastic calculation than in the previous cases and restraint stress becomes too high (Figure 6 and Figure 7). The end of the production of new phases occurs at about 180 days and free expansion stabilizes by this date (Figure 5). For restraint expansion, after the stabilization of expansion, a decrease of the restraint stress can be observed (Figure 6). It is due to the concrete relaxation, which is caused by the concrete viscoelastic behaviour, here, fitted on creep tests [41].

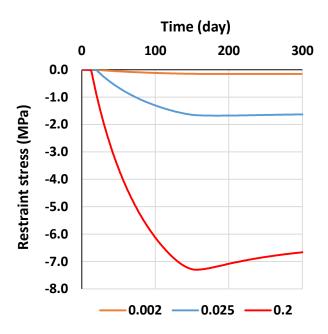


Figure 6: Restraint stress for an expansion of about 0.16% according to h_{crk}

In this paper, the calibration of the parameter h_{crk} has been performed to obtain a restraint stress of about 1 MPa for an expansion in stress-free conditions of about 0.1% (h_{crk} equal to 0.025). It is a usual mean value for expansive mechanisms under restraint. The modelling validation is performed in Figure 7 with the comparison with several experimental studies [30], [35], [36]. These works were performed for different initial materials and different new phases (ASR or ettringite). The modelling is able to evaluate the stress for restrained expansion of the three experimental studies, if expansion in stress-free condition is lower than 0.4%. A non-linear hardening law could give better results for larger expansions but the calculations would be more time-consuming (in cases of linear hardening, the implicit return mapping algorithm converges in one step only, which is no longer the case for nonlinear hardening). For phenomena with greater expansion (delayed ettringite formation, sulfate attack), a multi-linear description could lead to a more realistic evaluation without consuming too much computational time.

In some experiments, very small stress was noted for material with large potential for expansion in stress free conditions (Figure 7, [35]). It was due to exudation of products out of the specimens as observed by the authors of [35]. Such phenomena are not intrinsic

to the material and should not be reproduced by material modelling but by coupled modelling as proposed in [72]. Future works will combine the present modelling with transport modelling to reproduce such mechanisms.

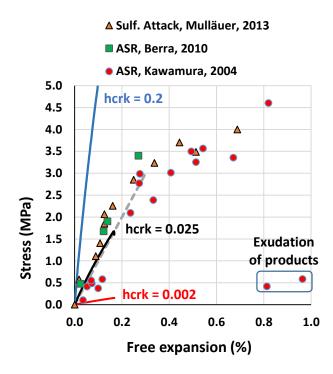


Figure 7: Restraint stress according to expansion in stress free condition, comparison with modelling according to h_{crk} (from 0.002 to 0.2), experimental data from [30], [35], [36]

4.3 Irreversibility of expansion during drying

The aim of this part is to analyse the ability of the model to reproduce the behaviour of concrete undergoing first expansion then drying shrinkage. After 650 days of expansion for the concrete analysed in part 3.1, specimens were exposed to air at 30% RH [50]. When the new phases due to alkali-silica reaction dried, their volume decreased because of water loss, but the concrete expansion did not change; only the usual concrete drying shrinkage occurred (Figure 8, [50]).

- For the calculations below, the same parameters as in part 3.1 are used for expansion.
- 538 Drying shrinkage is obtained through the Van Genuchten model [73] as explained in [41].
- 539 In this case, Equation (9) becomes:

$$\tilde{\sigma}_s = K_d \cdot (\varepsilon - \varepsilon_{an}) - \sum_a b_a \cdot p_a - b_w \cdot p_w$$
 (27)

- 540 with b_w , the Biot coefficient of water (dependent on the saturation degree of the porosity
- 541 in the material). p_w is the pressure due to water, which is negative in case of shrinkage
- 542 (due the capillarity effect) and zero during swelling in water. The pressure p_w is
- modelled using the Van Genuchten model [73]:

$$p_{w} = -M_{shr} \cdot \left(S_{r}^{-\frac{1}{m_{vg}}} - 1\right)^{(1 - m_{vg})} \tag{28}$$

- 544 M_{shr} and m_{vg} can be calibrated on the water retention curve or on the evolution of
- shrinkage strains.

- 547 In the present work, the Biot coefficient of water b_w has been evaluated from the
- 548 concrete porosity (16%) [74]. It is equal to 0.4 for this concrete in case of total saturation.
- 549 m_{vg} has been taken equal to the usual value 0.5, and only M_{shr} has to be calibrated. M_{shr}
- 550 is evaluated to reproduce the shrinkage strain on a concrete which has never been
- damaged by ASR (Figure 8-a). It is equal to 32 MPa, which is a usual value for concrete
- 552 [41]. The validation of the model is performed on the same concrete which is submitted
- 553 to the same drying but after ASR expansion (Figure 8-b). After expansion occurring in
- 554 water, concrete shrinks with the usual dependence on water pressure (Figure 8-b).
- 555 Cracking induced by the formation of the new phases did not change the amplitude of
- shrinkage significantly since the experimental results could be found without changing
- 557 the coefficients of Equations (27) and (28) after swelling. The decrease of ASR-gel
- volumes induced by the drying did not impact the irreversible expansion: they were either
- 559 filled by crystallized phases or were impossible to reclose simply because of the
- roughness of their lips. Figure 8-b shows that the behaviour observed on specimens can
- be reproduced by a basic combination of poromechanics (Equation (27)) with the linear
- anisotropic plasticity used in the constitutive equations.

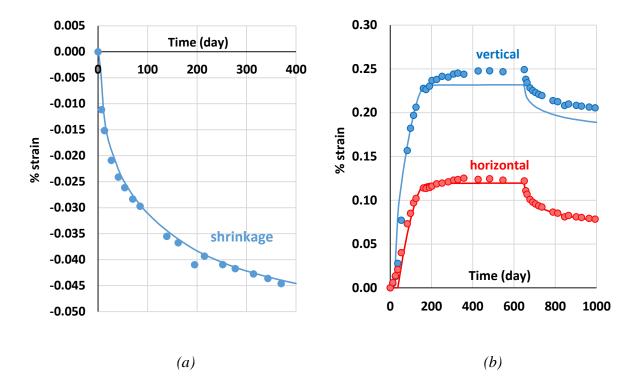


Figure 8: Calibration of shrinkage parameters on concrete which has never been damaged by ASR (a) and validation on the same concrete which is submitted to the same drying, after ASR expansion (b) (circles: experimental points [50], lines: modelling)

4.4 Damage due to pressure gradient

In the previous analysis, homogeneous conditions were assumed so as to analyse the response of the model from a material point of view without disturbance due to gradient effects. In reality, the specimens analysed just above were kept in water. Such storage leads to a pressure gradient due to alkali leaching: close to the specimen skin, alkalis leach out rapidly and cannot participate in the chemical reaction. As a result, chemical advancement is slower close to the skin than in specimen cores, which leads to pressure gradients and skin cracking. In the calculations, the risk of skin cracking and the cracks opening is evaluated by the model presented in [42]. The model is regularized with Hillerborg anisotropic method to avoid mesh dependence [75]. The calibration of the expansion curves in the two directions (Figure 9) is obtained for a molar volume of new phases, φ_{nv}^{mol} , equal to 22.1 cm³/mol, an average distance over which the new phases can

move without causing cracking, d_{ref} , equal to 7 μ m, and the anisotropy ratio, ρ_{ani} , equal to 0.82. The radial deformation is the radial displacement in P1 divided by the specimen radius, and the vertical deformation is the vertical displacement in P2 divided by the measurement basis (five centimetres above the symmetry axis as during experimentation – Figure 10). As a fraction of the reactants does not participate in the attack because of their leaching, the molar volume has to be slightly higher than in the previous calculations to obtain the same expansion. The gradient of advancement due to alkali leaching leads to the pressure gradient presented in Figure 10-a. Thus, tensile stresses at the external surface of concrete specimens (Figure 10-b) are sufficient to cause localized cracking with openings larger than 100 μ m (Figure 11), which is the cracking often observed on specimens in laboratory and real structures. Such a gradient can be induced by leaching or drying according to the environmental conditions (open cracks visible without microscopic tools, Figure 12) [1]. The diffuse cracking due to pressure is usually finer and forms a denser network (one or two cracks per aggregate [48]) and can also be observed on real structures sometimes (Figure 12).

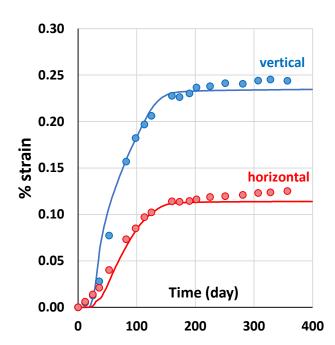


Figure 9: Comparison of calculated expansion and experimental data (circles: experimental points [50])

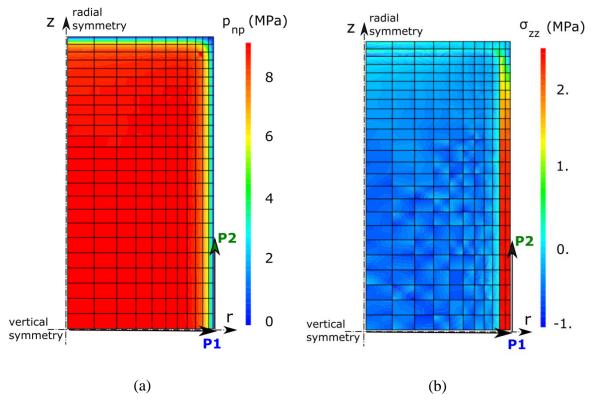


Figure 10: Pressure gradient due to alkali leaching (a) and induced stresses (b) just before skin cracking (in MPa)

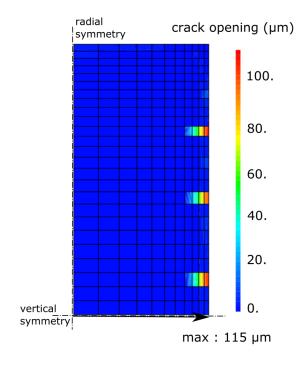


Figure 11: Cracking due to pressure gradient at the end of the test



Figure 12: Diffuse and localized cracks on column damaged by expansive phenomena

Investigations showed that expansive materials were usually subjected to a pressure gradient due to environmental conditions, even in laboratory tests performed on small specimens. Gradients of temperature, moisture or ionic species lead to gradients of pressure. Such gradients can lead to localized open cracks on the skin or in the core of specimens. This strongly impacts the expansion measurements and the consequences in terms of material damage evaluated on specimens. Diffuse and localized cracking do not have the same impact in terms of strength and rigidity decreases and of transfer properties. In the future, models will have to assess the crack opening due to pressure gradients in real structures as it will impact the durability of the structure through the induced modifications of transfer properties. Such an assessment can be performed from crack openings for localized cracks or for diffuse cracking. Therefore, modelling of expansive phenomena should be able to distinguish between diffuse damage due to pressure and localized damage due to gradient. In this work, the distinction is achieved by combining the plasticity modelling, used to represent the permanent strain due to diffuse

cracking induced by pressure presented above, with the damage modelling presented in [42].

4.5. Discussion

607

608

609

610

611

612

613

614

615

616

617

618

619

620

621

622

623

624

625

626

627

628

629

630

631

The previous calculations were performed in the framework of poromechanics. The Biot coefficient and modulus depend on the mechanical properties of the materials and on the volume of porosity filled by the new phases. For the multi-scale modelling used to assess the impact of alkali-silica reaction, the Biot coefficients of new phases in aggregate, evaluated through Equation (5), lie between 3.8e-2 (in homogeneous conditions) and 5.4e-2 (in the calculations with gradient) in the smallest aggregate (4/12) and between 1.8e-2 and 2.5e-2 in the largest one (12/20) at the end of the calculated expansion. These values are consistent with previous calculations performed for other new phases formed in concrete [12], [13]. The Biot coefficients of aggregate in concrete reach about 0.2 in the smaller aggregate (4/12) and 0.5 in the larger aggregates (4/12). This is consistent with modelling that evaluates the expansion from the action of the aggregate on the concrete [26], [61], [76] without representation of aggregate damage. It is usually performed in structural calculations. The modelling proposed in this paper makes the link between the two scales. Taking the shape of cracks into consideration could lead to slightly larger coefficients [26], [40]. This means that the present modelling could underestimate the percentage of expansion due to pressure and thus slightly overestimate the percentage due to cracking. Pressure due to the formation of new phases and evaluated by the present modelling lies between 10 and 15 MPa. These values are consistent with usual values measured for such new phases [77], [78] or evaluated through theoretical approaches [79], [80]. It is also a validation of the mechanical developments proposed in this paper.

5. Conclusion

- 633 The main consequences of expansion in quasi-brittle materials are: anisotropic induced
- cracking due to natural causes or due to external loading, stress for restrained expansion,
- 635 irreversibility of diffuse cracking and localized cracks due to pressure gradients.
- 636 A model of expansion in quasi-brittle materials has been proposed. It is based on
- poromechanics and on a plastic, anisotropic criterion to represent permanent strain due to
- 638 diffuse cracking caused by pressure. Thus the anisotropy of cracking is induced by the
- 639 addition of local stress due to pressure and external loading. Equations have been
- 640 proposed for multiple pressures to take account of the effects of differences of
- advancement in the formation of new products on pressure and induced damage.
- The following physical phenomena can be reproduced by the model:
- Anisotropy of expansion and cracking due to the initial anisotropy properties of
- the material,
- Induced stress in conditions of restraint,
- Irreversibility of expansion during drying periods,
- Shrinkage of cracked drying concrete previously affected by expansion,
- Combination of diffuse damage due to expansion and localized damage due to
- 649 gradient.
- The importance of diffuse cracking in the mechanisms of expansion in concrete has been
- 651 highlighted. This mechanical behaviour is strongly dependent on the mechanical
- 652 properties of the material subjected to expansion and particularly to properties in tension:
- 653 first for the diffuse damage and the direction of cracking due to pressure and, second, for
- 654 the localized cracks due to pressure gradient. The latter point introduces the
- quantification of localized crack opening to evaluate the consequences of damage due to
- 656 a skin gradient in terms of mechanical and transfer properties. Cracks are usually
- observed along reinforcements in structures subjected to expansion. These cracks shorten
- 658 the service life of damaged structures and the reduction can be evaluated from the crack
- opening. This is an important issue when modelling the durability of structures affected
- 660 by expansion.

6. References

- 663 [1] B. Fournier and M.-A. Bérubé, "Alkali-aggregate reaction in concrete: A review of basic concepts and engineering implications," *Can. J. Civ. Eng.*, vol. 27, pp. 167–191, 2000.
- 666 [2] S. Diamond, "Delayed ettringite formation Processes and problems," *Cem. Concr. Compos.*, vol. 18, pp. 205–215, 1996.
- 668 [3] C. Ouyang, A. Nanni, and W. F. Chang, "Internal and external sources of sulfate ions in Portland cement mortar; two types of chemical attack," *Cem. Concr. Res.*, vol. 18, pp. 699–709, 1988.
- 671 [4] M. Neji, B. Bary, P. Le Bescop, and N. Burlion, "Swelling behavior of ion exchange resins incorporated in tri-calcium silicate cement matrix: I. Chemical analysis," *J. Nucl. Mater.*, vol. 467, pp. 544–556, 2015.
- 674 [5] C. Huang and R. Feldman, "Dependence of Frost Resistance on the Pore Structure of Mortar Containing Silica Fume," *ACI J.*, vol. 82, no. 5, pp. 740–743, 1985.
- 676 [6] O. Coussy, *Poromechanics*, Wiley. New York, 2004.
- [7] L. Dormieux, D. Kondo, and F. Ulm, *Microporomechanics*, Wiley. 2006.
- 678 [8] J. Lubliner, J. Oliver, S. Oller, and E. Onate, "A plastic-damage model for concrete," *Int. J. Solids Struct.*, vol. 25, no. 3, pp. 299–326, 1989.
- 680 [9] A. D. Jefferson, "Craft a plastic-damage-contact model for concrete . I . Model theory and thermodynamic considerations," *Int. J. Solids Struct.*, vol. 40, pp. 5973–5999, 2003.
- 683 [10] B. Capra and A. Sellier, "Orthotropic modelling of alkali-aggregate reaction in concrete structures: numerical simulations," *Mech. Mater.*, vol. 6, no. December, 2002.
- 686 [11] E. Grimal, A. Sellier, Y. Le Pape, and E. Bourdarot, "Creep, Shrinkage, and Anisotropic Damage in Alkali-Aggregate Reaction Swelling Mechanism-Part I. A Constitutive Model," *ACI Mater. J.*, vol. 105, no. 3, pp. 227–235, 2008.
- 689 [12] B. Bary, N. Leterrier, E. Deville, and P. Le Bescop, "Coupled chemo-transport-690 mechanical modelling and numerical simulation of external sulfate attack in 691 mortar," *Cem. Concr. Compos.*, vol. 49, pp. 70–83, 2014.
- 692 [13] B. Bary, "Simplified coupled chemo-mechanical modeling of cement pastes behavior subjected to combined leaching and external sulfate attack," *Int. J. Numer. Anal. Methods Geomech.*, vol. 32, no. February, pp. 1791–1816, 2008.
- 695 [14] R. J. Flatt and G. W. Scherer, "Thermodynamics of crystallization stresses in DEF," *Cem. Concr. Res.*, vol. 38, pp. 325–336, 2008.
- 697 [15] R. Tixier and B. Mobasher, "Modeling of Damage in Cement-Based Materials Subjected to External Sulfate Attack . I: Formulation," *ASCE J. Mater. Civ. Eng.*,

- 699 vol. 15, no. August, pp. 305–313, 2003.
- 700 [16] A. E. Idiart, C. M. López, and I. Carol, "Chemo-mechanical analysis of concrete cracking and degradation due to external sulfate attack: A meso-scale model," *Cem. Concr. Compos.*, vol. 33, pp. 411–423, 2011.
- 703 [17] S. Sarkar, S. Mahadevan, J. C. L. Meeussen, H. Van Der Sloot, and D. S. Kosson, 704 "Numerical simulation of cementitious materials degradation under external 705 sulfate attack," *Cem. Concr. Compos.*, vol. 32, no. 3, pp. 241–252, 2010.
- 706 [18] N. Cefis and C. Comi, "Chemo-mechanical modelling of the external sulfate attack in concrete," *Cem. Concr. Res.*, vol. 93, pp. 57–70, 2017.
- 708 [19] A. Gholizadeh, F. Rajabipour, and J. L. Rosenberger, "Composition rheology relationships in alkali silica reaction gels and the impact on the gel's deleterious behavior," *Cem. Concr. Res.*, vol. 83, pp. 45–56, 2016.
- 711 [20] W. Puatatsananon and V. Saouma, "Chemo-mechanical micromodel for alkalisilica reaction," *ACI Mater. J.*, vol. 110, no. 110, pp. 67–77, 2013.
- 713 [21] M. Alnaggar, G. Cusatis, and G. Di Luzio, "Lattice Discrete Particle Modeling (LDPM) of Alkali Silica Reaction (ASR) deterioration of concrete structures," *Cem. Concr. Compos.*, vol. 41, pp. 45–59, 2013.
- 716 [22] G. W. Scherer, "Crystallization in pores," *Cem. Concr. Res.*, vol. 29, no. December 1998, pp. 1347–1358, 1999.
- 718 [23] O. Coussy, "Deformation and stress from in-pore drying-induced crystallization of salt," *J. Mech. Phys. Solids*, vol. 54, pp. 1517–1547, 2006.
- 720 [24] O. Coussy, "Poromechanics of freezing materials," *J. Mech. Phys. Solids*, vol. 53, pp. 1689–1718, 2005.
- 722 [25] Q. Zeng, T. Fen-Chong, P. Dangla, and K. Li, "A study of freezing behavior of cementitious materials by poromechanical approach," *Int. J. Solids Struct.*, vol. 48, no. 22–23, pp. 3267–3273, 2011.
- 725 [26] L. Charpin and A. Ehrlacher, "Microporomechanics study of anisotropy of ASR under loading," *Cem. Concr. Res.*, vol. 63, pp. 143–157, 2014.
- 727 [27] A. Sellier, J. P. Bournazel, and A. Mébarki, "Une modélisation de la réaction alcalis-granulat intégrant une description des phénomènes aléatoires locaux," 729 *Mater. Struct.*, vol. 28, no. 1, pp. 373–383, 1995.
- 730 [28] L. Charpin and A. Ehrlacher, "Simplified model for the transport of Alkali-Silica Reaction gel in concrete porosity," *J. Adv. Concr. Technol.*, vol. 12, pp. 1–6, 2014.
- 732 [29] Z. Bažant and S. Rahimi-Aghdam, "Diffusion-Controlled and Creep-Mitigated ASR Damage via Microplane Model . I : Mass Concrete," *J. Eng. Mech.*, vol. 143, no. 3, pp. 1–10, 2017.
- 735 [30] W. Müllauer, R. E. Beddoe, and D. Heinz, "Sulfate attack expansion mechanisms," *Cem. Concr. Res.*, vol. 52, pp. 208–215, 2013.
- 737 [31] T. Ichikawa, "Alkali-silica reaction, pessimum effects and pozzolanic effect," 738 *Cem. Concr. Res.*, vol. 39, pp. 716–726, 2009.

- 739 [32] T. Ichikawa and M. Miura, "Modified model of alkali-silica reaction," *Cem. Concr. Res.*, vol. 37, pp. 1291–1297, 2007.
- 741 [33] E. Garcia-Diaz, J. Riche, D. Bulteel, and C. Vernet, "Mechanism of damage for the alkali-silica reaction," *Cem. Concr. Res.*, vol. 36, pp. 395–400, 2006.
- 743 [34] E. Garcia-Diaz, D. Bulteel, Y. Monnin, P. Degrugilliers, and P. Fasseu, "ASR pessimum behaviour of siliceous limestone aggregates," *Cem. Concr. Res.*, vol. 40, no. 4, pp. 546–549, 2010.
- 746 [35] M. Kawamura and K. Iwahori, "ASR gel composition and expansive pressure in mortars under restraint," *Cem. Concr. Compos.*, vol. 26, pp. 47–56, 2004.
- 748 [36] M. Berra, G. Faggiani, T. Mangialardi, and a. E. Paolini, "Influence of stress restraint on the expansive behaviour of concrete affected by alkali-silica reaction," *Cem. Concr. Res.*, vol. 40, pp. 1403–1409, 2010.
- 751 [37] H. Kagimoto, Y. Yasuda, and M. Kawamura, "ASR expansion, expansive pressure and cracking in concrete prisms under various degrees of restraint," *Cem. Concr. Res.*, vol. 59, pp. 1–15, 2014.
- 754 [38] H. Bouzabata, S. Multon, A. Sellier, and H. Houari, "Effects of restraint on expansion due to delayed ettringite formation," *Cem. Concr. Res.*, vol. 42, no. 7, pp. 1024–1031, 2012.
- 757 [39] K. Mori and K. Tanaka, "Average stress in matrix and average elastic energy of materials with misfitting inclusions," *Acta Mettalurg.*, vol. 21, no. 5, pp. 1605–1609, 1973.
- 760 [40] R. Esposito and M. A. N. Hendriks, "A multiscale micromechanical approach to
 761 model the deteriorating impact of alkali-silica reaction on concrete," *Cem. Concr. Compos.*, vol. 70, pp. 139–152, 2016.
- 763 [41] A. Sellier, S. Multon, L. Buffo-Lacarrière, T. Vidal, X. Bourbon, and G. Camps, 764 "Concrete creep modelling for structural applications: non-linearity, multi-axiality, 765 hydration, temperature and drying effects," *Cem. Concr. Res.*, vol. 79, pp. 301– 766 315, 2016.
- 767 [42] A. Sellier, G. Casaux-Ginestet, L. Buffo-Lacarrière, and X. Bourbon, "Orthotropic Damage Coupled with Localised Crack Reclosure Processing. Part I: Constitutive Laws," *Eng. Fract. Mech.*, vol. 97l, no. January, pp. 148–167, Oct. 2013.
- 770 [43] C. Larive, "Apports combinés de l'expérimentation et de la modélisation à la compréhension de l'alcali-réaction et de ses effets mécaniques, Laboratoire Central des Ponts et Chaussées (Edt.), Ouvrage d'Art, Rapport OA 28," 1998.
- 773 [44] F.-J. Ulm, O. Coussy, K. Li, and C. Larive, "Thermo-Chemo-Mechanics of ASR expansion in concrete structures," *ASCE J. Eng. Mech.*, vol. 126, no. March, pp. 233–242, 2000.
- 776 [45] J. Berard, R. Roux, I. Depuis, and C. Climinces, "La viabilite des betons du Quebec: le role des granulats," *Can J Civ Eng*, vol. 13, no. 1, pp. 12–24, 1986.
- 778 [46] J. M. Ponce and O. R. Batic, "Different manifestations of the alkali-silica reaction

- in concrete according to the reaction kinetics of the reactive aggregate," *Cem. Concr. Res.*, vol. 36, pp. 1148–1156, 2006.
- 781 [47] M. Ben Haha, E. Gallucci, A. Guidoum, and K. L. Scrivener, "Relation of expansion due to alkali silica reaction to the degree of reaction measured by SEM image analysis," *Cem. Concr. Res.*, vol. 37, pp. 1206–1214, 2007.
- 784 [48] L. F. M. Sanchez, B. Fournier, M. Jolin, and J. Duchesne, "Reliable quantification of AAR damage through assessment of the Damage Rating Index (DRI)," *Cem. Concr. Res.*, vol. 67, pp. 74–92, 2015.
- 787 [49] A. B. Giorla, K. L. Scrivener, and C. F. Dunant, "Influence of visco-elasticity on the stress development induced by alkali–silica reaction," *Cem. Concr. Res.*, vol. 70, pp. 1–8, 2015.
- 790 [50] S. Multon and F. Toutlemonde, "Effect of moisture conditions and transferts on alkali silica reaction damaged structures," *Cem. Concr. Res.*, vol. 40, pp. 924–934, 2010.
- 793 [51] N. Smaoui, M.-A. Bérubé, B. Fournier, and B. Bissonnette, "Influence of Specimen Geometry, Orientation of Casting Plane, and Mode of Concrete Consolidation on Expansion Due to ASR," *Cem. Concr. Aggregates*, vol. 26, no. 2, pp. 1–13, 2004.
- 797 [52] G. Wardeh and B. Perrin, "Freezing-thawing phenomena in fired clay materials and consequences on their durability," *Constr. Build. Mater.*, vol. 22, pp. 820–828, 2008.
- 800 [53] C. Larive, M. Joly, and O. Coussy, "Heterogeneity and anisotropy in ASR-affected concrete –Consequences for structural assessment," in *11th International Conference on Alkali-Aggregate Reaction in Concrete*, 2000, pp. 969–978.
- 803 [54] S. Multon and F. Toutlemonde, "Effect of applied stresses on alkali-silica reaction-induced expansions," *Cem. Concr. Res.*, vol. 36, no. 5, pp. 912–920, 2006.
- 805 [55] C. F. Dunant and K. L. Scrivener, "Effects of uniaxial stress on alkali-silica reaction induced expansion of concrete," *Cem. Concr. Res.*, vol. 42, no. 3, pp. 567–576, 2012.
- 808 [56] B. P. Gautam, D. K. Panesar, S. A. Sheikh, and F. J. Vecchio, "Multiaxial Expansion-Stress Relationship for Alkali Silica Reaction-Affected Concrete," *ACI Mater. J.*, vol. 114, no. 1, pp. 171–184, 2017.
- J. Liaudat, I. Carol, C. M. López, and V. E. Saouma, "ASR expansions in concrete under triaxial confinement," *Cem. Concr. Compos.*, vol. doi: 10.10, 2017.
- H. Kagimoto and M. Kawamura, "Measurements of strain and humidity within massive concrete cylinders related to the formation of ASR surface cracks," *Cem. Concr. Res.*, vol. 41, pp. 808–816, 2011.
- 816 [59] R.-P. Martin, "Analyse sur structures modèles des effets mécaniques de la réaction sulfatique interne du béton, Ph.D. thesis, LCPC Laboratoire Central des Ponts et Chaussées Paris," 2010.

- 819 [60] M. Salgues, "Modélisations des effets structuraux des réactions sulfatiques 820 internes et alcali-granulats: Application aux barrages en béton, PhD Thesis, 821 Université de Toulouse," 2013.
- 822 [61] P. Morenon, S. Multon, A. Sellier, E. Grimal, F. Hamon, and E. Bourdarot, "Impact of stresses and restraints on ASR expansion," *Constr. Build. Mater.*, vol. 140, pp. 58–74, 2017.
- 825 [62] J. Simo, *Numerical analysis and simulation of plasticity*. Ciarlet, P., Lions, J. 826 (Eds.), Handbook of Numerical Analysis, vol. VI. North- Holland, 1998.
- 827 [63] S. Multon and A. Sellier, "Multi-scale analysis of alkali-silica reaction (ASR): 828 Impact of alkali leaching on scale effects affecting expansion tests," *Cem. Concr.* 829 *Res.*, vol. 81, pp. 122–133, 2016.
- 830 [64] A. Leemann and P. Lura, "E-modulus of the alkali-silica-reaction product determined by micro-indentation," *Constr. Build. Mater.*, vol. 44, pp. 221–227, 2013.
- C. Zhang, L. Sorelli, B. Fournier, J. Duchesne, J. Bastien, and Z. Chen, "Stress-relaxation of crystalline alkali-silica reaction products: Characterization by microand nanoindentation and simplified modeling," *Constr. Build. Mater.*, vol. 148, pp. 455–464, 2017.
- M. Kawamura and H. Fuwa, "Effects of lithium salts on ASR gel composition and expansion of mortars," *Cem. Concr. Res.*, vol. 33, pp. 913–919, 2003.
- 839 [67] S. Goto and D. M. Roy, "Diffusion of ions through hardened cement pastes," *Cem. Concr. Res.*, vol. 11, pp. 751–757, 1981.
- 841 [68] T. Kim, J. Olek, and H. Jeong, "Alkali–silica reaction: Kinetics of chemistry of pore solution and calcium hydroxide content in cementitious system," *Cem. Concr. Res.*, vol. 71, pp. 36–45, 2015.
- 844 [69] A. Perruchot, P. Massard, and J. Lombardi, "Composition et volume molaire apparent des gels Ca–Si, une approche expérimentale," *C. R. Geosci.*, vol. 335, pp. 951–958, 2003.
- K. L. Scrivener and K. M. Nemati, "The percolation of pore space in the cement paste/aggregate interfacial zone of concrete," *Cem. Concr. Res.*, vol. 26, no. 1, pp. 35–40, 1996.
- K. L. Scrivener, A. K. Crumbie, and P. Laugesen, "The interfacial transition zone (ITZ) between cement paste and aggregate in concrete," *Interface Sci.*, vol. 12, no. 4, pp. 411–421, 2004.
- 853 [72] Y. Takahashi, S. Ogawa, Y. Tanaka, and K. Maekawa, "Scale-Dependent ASR Expansion of Concrete and Its Prediction coupled with Silica Gel Generation and Migration," *J. Adv. Concr. Technol.*, vol. 14, pp. 444–463, 2016.
- T. M. Van Genuchten and D. Nielsen, "On describing and predicting the hydraulic properties of unsaturated soils," *Ann. Phys.*, vol. 3, no. 5, pp. 615–628, 1985.
- 858 [74] B. Zuber and J. Marchand, "Modeling the deterioration of hydrated cement

- systems exposed to frost action Part 1: Description of the mathematical model," *Cem. Concr. Res.*, vol. 30, no. 2000, pp. 1929–1939, 2000.
- A. Hillerborg, M. Modéer, and P.-E. Petersson, "Analysis of crack formation and crack growth in concrete by means of fracture mechanics and finite elements," *Cem. Concr. Res.*, vol. 6, pp. 773–782, 1976.
- 864 [76] C. Comi, B. Kirchmayr, and R. Pignatelli, "Two-phase damage modeling of concrete affected by alkali silica reaction under variable temperature and humidity conditions," *Int. J. Solids Struct.*, vol. 49, no. 23–24, pp. 3367–3380, 2012.
- 868 [77] L. J. Stuble and S. Diamond, "Swelling Properties of Synthetic Alkali Silica Gels," 869 *J. Am. Ceram. Soc.*, vol. 64, no. 11, pp. 652–655, 1981.
- 870 [78] H. W. Reinhardt and O. Mielich, "A fracture mechanics approach to the crack formation in alkali-sensitive grains," *Cem. Concr. Res.*, vol. 41, no. 3, pp. 255–262, 2011.
- 873 [79] M. Prezzi, P. J. M. Monteiro, and G. Sposito, "The alkali-silica reaction, part I: Use of the double-layer theory to explain the behavior of reaction-product gels," *ACI Mater. J.*, vol. 94, no. 94, pp. 10–17, 1997.
- 876 [80] R. Pignatelli, C. Comi, and P. J. M. Monteiro, "A coupled mechanical and chemical damage model for concrete affected by alkali-silica reaction," *Cem. Concr. Res.*, vol. 53, pp. 196–210, 2013.