

An inverse analysis approach for the identification of the hygro-thermo-chemical model parameters of concrete

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Abstract

Hygro-thermo-chemical models provide useful representations of the mechanisms of moisture transport and temperature variations that take place in concrete structures and that can influence their durability and service behaviour. Several material parameters need to be specified when performing a hygro-thermo-chemical simulation. While some of these parameters can be evaluated based on the concrete mix specifications or from data reported in the literature, some other parameters are not readily available from the literature, partly because of their large variability and partly because they do not possess a precise physical meaning. In this context, this paper presents a robust inverse analysis procedure for the identification of this latter set of material parameters. The inverse analysis problem is formulated by using temperature and relative humidity profiles taking place within a concrete component as input. The proposed approach is applied to evaluate the minimum number of temperature and relative humidity measurements that are necessary to be performed for a successful identification of the sought material parameters. Representative results of an extensive sensitivity analysis are presented to gain insight into the most effective locations within the concrete component for the measurements and instants in time when these measurements should be collected. The inverse analysis procedure is then presented and

28 validated against a set of pseudo-experimental results affected by different levels of noise,
29 highlighting the robustness of the proposed methodology when applied with the arrangements
30 suggested in terms of discrete relative humidity and temperature measurements and monitoring
31 periods.

32

33 **Keywords**

34 Concrete; Hygro-thermo-chemical model; Identifiability; Inverse analysis; Model parameter
35 characterisation

36

37 **1. Introduction**

38 Durability and serviceability limit states represent important requirements associated with the
39 design of concrete structures. Excessive deformations, displacements and cracks may
40 drastically affect the service behaviour of a structure and lead to increased maintenance costs.
41 These effects are influenced by the time-dependent properties of the concrete and, in particular,
42 by the physical and chemical mechanisms that take place in the concrete, especially in its early
43 age. Moisture transport during hardening, occurring for release of water through the external
44 surfaces and for internal water consumption due to chemical reactions such as cement
45 hydration, causes volume changes that give rise to drying and autogenous shrinkage strains,
46 respectively. The heat released during the cement hydration reaction may also cause volume
47 changes inside the concrete. Different numerical and experimental studies on the early concrete
48 behaviour exist in the literature and deal with the self-heating and self-drying phenomena.
49 Bažant and Najjar [1] proposed a well-known material model for nonlinear moisture transport
50 suitable for concrete and similar materials. This model was extended in subsequent years, for
51 example, by including the direct modelling of the cement hydration occurring in concrete at
52 early age by means of a thermodynamics based approach (e.g. [2]); by considering the aging
53 effect on strength development through a coupled thermo-chemo-mechanical model (e.g. [3])
54 or, more recently, by taking into account the permeability increase once a macro crack is
55 formed (e.g. [4]). Kim and Lee [5] and Oh and Cha [6] proposed a model for moisture and
56 temperature calculation at concrete early age, where a sink term was added to the diffusive
57 moisture equation to account for internal water consumption. A multi-phase coupled thermo-
58 chemo-mechanical model was proposed by Gawin [7] and more recently by Du [8] and it
59 accounted for the porous nature of the concrete by considering a micro-scale description of the
60 material. The effects of the 3D meso-structure, modelled with different aggregate particles
61 shapes and porous cement paste matrix, and of microcracks distribution on diffusivity and

62 permeability of concrete materials has been studied in [9] and [10]. A new cement hydration
63 model has been proposed in [11], considering the effects of C-S-H layers forming around
64 anhydrous cement grains to control the very long hydration process which may occur in thick
65 concrete components. Di Luzio et al. ([12] and [13]) proposed a hygro-thermo-chemical model
66 by considering the effect of cement hydration on both moisture and temperature calculations in
67 terms of internal water consumption and self-heating generation.

68 While the use of such hygro-thermo-chemical models provides great insight into the material
69 behaviour, it requires the knowledge and input of several material parameters. The latter can be
70 subdivided into two major sets: (i) one set of parameters that can be evaluated based on the
71 concrete mix specifications or from data reported in the literature; and (ii) a second set of
72 parameters that are characterised by a large variability (based on data available in the literature)
73 and, among these, many parameters do not possess a precise physical meaning and, for this
74 reason, are not amenable to a direct measurement. The inability of the latter set of parameters
75 to be easily identified provides a limitation on the wider use of the hygro-thermo-chemical
76 model.

77 In this context, this paper aims to provide a robust procedure for the identification of the set of
78 material parameters for the hygro-thermo-chemical modelling defined at point (ii), i.e.
79 parameters characterised by a large variability, some of which not amenable to a direct
80 measurement because not reflecting a precise physical property. The proposed approach relies
81 on the use of an inverse analysis procedure (see [14], [15] and [16]) that adopts temperature
82 and relative humidity distributions as input data. The particularity of the proposed
83 methodology is to give indication on the minimum number of temperature and relative
84 humidity measurements that are required for a successful identification of the material
85 parameters. This minimum requirement is established after evaluating through an extensive
86 sensitivity analysis (of which representative results are presented in the following) the most

87 effective locations and instants from concrete casting for the temperature and relative humidity
88 measurements to take place through the thickness of a typical concrete component. The
89 identification of the optimal locations and instants in time for the temperature and humidity
90 measurements has significant practical implications, because supporting the effective planning
91 of monitoring and measurement setups for laboratory or in-situ investigations. This becomes
92 particularly significant considering the fact that recent technological advancements have led to
93 a growing use and acceptance of temperature and relative humidity sensors embedded in
94 concrete [17], for example, for its real-time strength monitoring. The outcomes of the proposed
95 study will enable to optimise the number, locations and durations of the measurements while
96 maximising the information collected.

97 In the first part of the paper, the hygro-thermo-chemical model is presented. In this section, a
98 clear distinction is provided between the sets of parameters required by this model that can be
99 determined from either the concrete mix specifications or from data available in the literature,
100 and those that are characterised by a large variability and that are the focus of the present study.
101 In view of using recorded temperature and relative humidity information as input in the inverse
102 analysis process, the influence and responsiveness of the different material parameters on these
103 two fields is discussed and representative trends are reported. The inverse analysis procedure is
104 then introduced and its robustness is tested considering different scenarios constructed using
105 pseudo-experimental data subjected to different degrees of noise. Representative results are
106 provided to highlight the robustness of the proposed methodology when applied with the
107 arrangements suggested for the discrete relative humidity and temperature measurements and
108 with the recommended monitoring periods.

109 2. Hygro-thermo-chemical model

110 This section presents the hygro-thermo-chemical model capable to describe, over a spatial
111 domain Ω , how the variations of the relative humidity h and temperature T take place over time
112 t in a concrete component while accounting for different environmental conditions.

113 The model here adopted has been proposed in [12] and here applied, without any loss of
114 generality, to a concrete mix without the presence of silica fume. The water transport
115 mechanisms taking place in the concrete are described by the combination of the Fick's law,
116 expressing the flux of water mass \mathbf{j} as proportional to the gradient of the relative humidity h
117 (i.e. $\mathbf{j} = -D_h \nabla h$) and the water mass balance equation, e.g. [1-12]:

$$\frac{\partial w}{\partial t} = \nabla \cdot [D_h \nabla h] \quad \text{in } \Omega \quad (1)$$

118 where the total water content w depicts the sum of the evaporable water w_e and the non-
119 evaporable water w_n , i.e. the water chemically bonded, for example, by cement hydration. The
120 moisture diffusion D_h depends on the relative humidity h and temperature T as highlighted by
121 the following expression [12]:

$$D_h(h, T) = \psi(T) D_1 \left[1 + \left(\frac{D_1}{D_0} - 1 \right) (1-h)^n \right]^{-1} \quad (2)$$

122 in which $\psi(T) (= e^{(E_{ad}/RT_0 - E_{ad}/RT)})$, with T_0 being the reference room temperature (taken
123 as $296^\circ K$ in the simulations presented in the following), considers the influence of the
124 temperature on the moisture diffusion (see [18]), while it is usually assumed that
125 $E_{ad}/R = 4700K$ (see e.g. [1]), and parameters D_0 , D_1 and n depend on the specific concrete
126 mix. In the literature, it is recognized that moisture diffusion depends on different transport
127 mechanisms, which can be modelled individually to achieve a more physical description of the

128 process. However, such an approach requires a series of information, such as concrete pore
 129 structure, pore radii and connectivity, that is usually not readily available or easily measurable
 130 from experimental tests. As this paper is focused at the identification of optimal or acceptable
 131 sets for practical experimental measurements, it is felt that the use of this single
 132 phenomenological law for the modelling of the different underlying physical mechanisms is
 133 acceptable, as also adopted by others in the literature [1,12].

134 Under the assumption that the non-evaporable water can be expressed as $w_n(\alpha_c) = k_c \alpha_c c$, with
 135 c being the cement ratio content and k_c a material parameter that, according to [12] and
 136 references herein, can be assumed equal to 0.253, and assuming the evaporable water to be
 137 expressed as a function of the relative humidity and of the degree of cement hydration α_c , i.e.
 138 $w_e = w_e(h, \alpha_c)$, Equation (1) can be rewritten as follows:

$$\frac{\partial w_e}{\partial h} \frac{\partial h}{\partial t} = \nabla \cdot [D_h \nabla h] - \left(\frac{\partial w_e}{\partial \alpha_c} + k_c c \right) \dot{\alpha}_c \quad \text{in } \Omega \quad (3)$$

139 where the dot operator represents partial differentiation with respect to time t and α_c is
 140 calculated as the ratio between the level of hydration X_c and its theoretical asymptotic value
 141 $X_c^{\infty,th}$ exhibited in ideal hygro-thermal conditions. The maximum level of hydration at time
 142 infinity X_c^∞ is usually assumed to remain below $X_c^{\infty,th}$ and, therefore, the maximum value of
 143 the reaction degree $\alpha_c^\infty = X_c^\infty / X_c^{\infty,th}$ is usually smaller than one, i.e. $\alpha_c^\infty < 1$. According to [19],
 144 we may assume $\alpha_c^\infty = (1.032 w/c) / (0.194 + w/c)$, with w/c being the water-to-cement ratio.

145 Equation (3) highlights how the local variation of humidity depends on the divergence of the
 146 moisture flux and on two additional terms describing the microstructure variation (gel
 147 formation) and the internal consumption due to cement hydration.

148 The variation of α_c over time increases with relative humidity content and reduces while
 149 approaching its asymptotic value α_c^∞ as described by:

$$\alpha_c = A_{c1} \left(\frac{A_{c2}}{\alpha_c^\infty} + \alpha_c \right) \cdot (\alpha_c^\infty - \alpha_c) \cdot e^{\left(-\frac{\eta_c \alpha_c}{\alpha_c^\infty} \right)} \cdot \frac{1}{\left[1 + (a - ah)^b \right]} \cdot e^{\left(-\frac{\gamma_c}{T} \right)} \quad (4)$$

150 where $\gamma_c = E_{ac}/R$ with E_{ac} being the hydration activation energy and R the universal gas
 151 constant. Parameters A_{c1} , A_{c2} and η_c have no precise physical meaning and govern the so-
 152 called normalized chemical affinity. Constants a and b enter into the empirical function
 153 $b_h(h) = \left[1 + (a - ah)^b \right]^{-1}$, which takes into account the slowing of the hydration process when
 154 relative humidity decreases below a certain value (around 80%). Their values are usually taken
 155 equal to $a = 7.5$ and $b = 4.0$ (see [1]).

156 The evaporable water can be expressed as a function of the relative humidity (sorption
 157 isotherm curve) as follows:

$$w_e(h, \alpha_c) = \kappa_{vg}^c \alpha_c c (1 - 1/\bar{e}_2) + \frac{w_0 - 0.188 \alpha_c c - \kappa_{vg}^c \alpha_c c (1 - 1/\bar{e}_1)}{(\bar{e}_1 - 1)} (\bar{e}_2 - 1) \quad (5)$$

158 in which w_0 ($= (w/c)c$) is the initial water content and it is assumed that

159 $\bar{e}_2 = e^{10(g_1 \alpha_c^\infty - \alpha_c)h}$ and $\bar{e}_1 = e^{10(g_1 \alpha_c^\infty - \alpha_c)}$. Equation (5) depends on two other material

160 parameters κ_{vg}^c and g_1 that govern the amount of water contained in the cement gel pores and

161 the shape of the sorption curve, respectively. From equation (5), the moisture capacity $\partial w_e / \partial h$

162 is derived and inserted in equation (3).

163 The temperature field is calculated based on the Fourier's law, in which the heat flux \mathbf{q} is
164 expressed as a function of the temperature spatial gradient ($\mathbf{q} = \lambda \nabla T$), and the enthalpy
165 balance equation as follows:

$$\rho c_t \frac{\partial T}{\partial t} = \nabla \cdot [\lambda \nabla T] + \dot{\mathcal{Q}}_c \quad \text{in } \Omega \quad (6)$$

166 where T is the absolute temperature, λ is the heat conductivity that can be assumed constant for
167 the temperature range considered in the present study, while ρ and c_t depict the concrete mass
168 density and the specific heat, respectively, and $\dot{\mathcal{Q}}_c$ represents the rate of heat generation due to
169 cement hydration, calculated as $\dot{\mathcal{Q}}_c = \alpha_c \dot{\mathcal{Q}}_c^0$, with $\dot{\mathcal{Q}}_c^0$ being the total heat content per unit
170 cement mass due to cement hydration.

171 Equations (3) and (6) are coupled by their dependency on the degree of cement hydration α_c
172 as well as by the moisture diffusion coefficient D_h that depends on both temperature and
173 relative humidity.

174 The hygro-thermo-chemical model depends on a series of parameters. Some of them are well
175 known concrete characteristics, whose values can be evaluated based on the concrete mix
176 specifications or from data reported in the literature. These parameters are listed in the upper
177 part of Table 1. Other parameters are characterised by a large variability (considering data
178 available in the literature) and, among these, some do not possess a precise physical meaning.
179 This set of parameters is listed in the lower part of Table 1 and their range of variation
180 (obtained and derived from [12, 13, 20 and 21]) is collected in Table 2.

181

182 Table 1.

183

184 Table 2.

185

186

Table 3.

187

188 **2.1 Finite element formulation**

189 The hygro-thermo-chemical model described in Equations (3) and (6) is solved in the
 190 following by means of the finite element method, giving rise to the following discretized
 191 equations:

$$\begin{cases} \mathbf{W}\dot{\mathbf{H}} + \mathbf{D}\mathbf{H} = \mathbf{F} \\ \mathbf{C}\dot{\mathbf{T}} + \mathbf{\Lambda}\mathbf{T} = \mathbf{Q} \end{cases} \quad (7)$$

192 where \mathbf{H} and \mathbf{T} depict unknown vectors that collect all nodal values (of the finite element
 193 representation) of the relative humidity and temperature fields at each instant, while the system
 194 matrices are defined as:

$$\mathbf{W} = \bigcup_e \int_{\Omega_e} \mathbf{N}_e^T \frac{\partial w_e}{\partial h} \mathbf{N}_e d\Omega \quad (8)$$

$$\mathbf{D} = \bigcup_e \int_{\Omega_e} \mathbf{B}_e^T D_h \mathbf{B}_e d\Omega \quad (9)$$

$$\mathbf{F} = -\bigcup_e \int_{\Gamma_e} \mathbf{N}_e^T \mathbf{n}^T \mathbf{j} d\Gamma - \bigcup_e \int_{\Omega_e} \mathbf{N}_e^T \left(\frac{\partial w_e}{\partial \alpha_c} + 0.253c \right) \dot{\alpha}_c d\Omega \quad (10)$$

$$\mathbf{C} = \bigcup_e \int_{\Omega_e} \mathbf{N}_e^T \rho c_r \mathbf{N}_e d\Omega \quad (11)$$

$$\mathbf{\Lambda} = \bigcup_e \int_{\Omega_e} \mathbf{B}_e^T \lambda \mathbf{B}_e d\Omega \quad (12)$$

$$\mathbf{Q} = -\bigcup_e \int_{\Gamma_e} \mathbf{N}_e^T \mathbf{n}^T \mathbf{q} d\Gamma + \bigcup_e \int_{\Omega_e} \mathbf{N}_e^T \dot{\mathcal{Q}}_c d\Omega \quad (13)$$

195 where symbol \bigcup_e refers to the assembly operation typical of the finite element approach, and

196 matrices \mathbf{N}_e and \mathbf{B}_e collect shape functions and their spatial derivatives, respectively.

197 For the solution of Equations (7), Dirichlet's boundary conditions (on h and T) are directly
 198 imposed on the unknown vectors \mathbf{H} and \mathbf{T} , while Cauchy's boundary conditions can be
 199 introduced in the right end side of the equation, see [22].

200 Equation (7) can be integrated over time by means of the so-called θ -method [22]:

$$\left\{ \begin{array}{l} \left[\theta \mathbf{W}^{k+1} + (1-\theta) \mathbf{W}^k \right] \frac{\mathbf{H}^{k+1} - \mathbf{H}^k}{\Delta t} + \\ \quad \left[\theta \mathbf{D}^{k+1} + (1-\theta) \mathbf{D}^k \right] \left[\theta \mathbf{H}^{k+1} + (1-\theta) \mathbf{H}^k \right] = \left[\theta \mathbf{F}^{k+1} + (1-\theta) \mathbf{F}^k \right] \\ \left[\theta \mathbf{C}^{k+1} + (1-\theta) \mathbf{C}^k \right] \frac{\mathbf{T}^{k+1} - \mathbf{T}^k}{\Delta t} + \\ \quad \left[\theta \mathbf{\Lambda}^{k+1} + (1-\theta) \mathbf{\Lambda}^k \right] \left[\theta \mathbf{T}^{k+1} + (1-\theta) \mathbf{T}^k \right] = \left[\theta \mathbf{Q}^{k+1} + (1-\theta) \mathbf{Q}^k \right] \end{array} \right. \quad (14)$$

201 The above equations are approximated by taking the system matrices and the "load" vector at
 202 the previous instant k and by assuming $\theta = 1/2$ for the remaining term:

$$\left\{ \begin{array}{l} \mathbf{W}^k \frac{\mathbf{H}^{k+1} - \mathbf{H}^k}{\Delta t} + \mathbf{D}^k \frac{\mathbf{H}^{k+1} + \mathbf{H}^k}{2} = \mathbf{F}^k \\ \mathbf{C}^k \frac{\mathbf{T}^{k+1} - \mathbf{T}^k}{\Delta t} + \mathbf{\Lambda}^k \frac{\mathbf{T}^{k+1} + \mathbf{T}^k}{2} = \mathbf{Q}^k \end{array} \right. \quad (15)$$

203 These equations are then solved with respect to the unknown vectors at instant $k+1$:

$$\left\{ \begin{array}{l} \mathbf{H}^{k+1} = \left[\mathbf{W}^k + 1/2 \Delta t \mathbf{D}^k \right]^{-1} \left[\mathbf{W}^k \mathbf{H}^k + \Delta t \mathbf{F}^k - 1/2 \Delta t \mathbf{D}^k \mathbf{H}^k \right] \\ \mathbf{T}^{k+1} = \left[\mathbf{C}^k + 1/2 \Delta t \mathbf{\Lambda}^k \right]^{-1} \left[\mathbf{C}^k \mathbf{T}^k + \Delta t \mathbf{Q}^k - 1/2 \Delta t \mathbf{\Lambda}^k \mathbf{T}^k \right] \end{array} \right. \quad (16)$$

204 Time step Δt is not taken constant through the analysis but its value is increased as the
 205 simulation evolves since the rate of change of the mechanisms involved in the process
 206 decreases. In particular, after some convergence tests, Δt was taken equal to: 1200 s from the
 207 beginning to twice the curing time, then equal to 4 h up to 40 days, then 40 h up to 1 year and

208 then equal to 400 h up to the final time. Optimized time steps strategies could have been
209 investigated, in order to reduce the total computing time, but this was considered out of the
210 scope of the present publication.

211 The use of the proposed numerical model is illustrated by evaluating the variations over time of
212 the humidity profiles that occur in a typical concrete component exposed for drying and heat
213 exchange through its top and bottom surfaces (Figure 1). With reference to the initial
214 conditions adopted in the numerical analyses, at instant $t=0$ (instant of concrete casting and
215 beginning of the curing period) relative humidity and temperature are set equal to 100% and
216 296 K (room temperature), respectively, and the degree of cement hydration is assumed null.

217 Two types of boundary conditions are considered in this study and these reflect possible
218 conditions, such as those that could be specified in a laboratory environment when dealing with
219 shrinkage measurements of concrete specimens, see figure 1:

- 220 • Curing phase. As for the humidity field, all sides are sealed by the formworks except
221 for the upper side which is kept wet. For this reason on the lateral and lower sides of the
222 finite element model zero-Cauchy boundary conditions are imposed while a relative
223 humidity equal to 100% is assumed on the upper side of the model. These boundary
224 conditions for the humidity field produce the loss of symmetry in figure 2. For the
225 temperature field, it is assumed that the formworks are not able to impose perfect
226 adiabatic conditions and, for this reason, the room temperature is assumed on both the
227 upper and lower sides of the model. This selection of boundary conditions is preferred
228 to test the proposed inverse algorithm with respect to the most unfavourable conditions
229 because adiabatic conditions on the lower side would induce higher temperatures and,
230 therefore, pseudo-experimental information more sensitive to the sought parameters. On
231 the lateral sides of the finite element model adiabatic conditions are assumed.

232 • Drying phase. After the curing period, the lateral sides are sealed, for example, with
233 plastic sheets to achieve relative humidity and heat fluxes along one direction only, i.e.
234 along the thickness of the concrete component. For this reason, on the lateral
235 boundaries of the finite element model zero-Cauchy boundary conditions are imposed,
236 while on the upper and lower sides Dirichlet boundary conditions that enable heat and
237 moisture exchange are imposed, as indicated in figure 1. These boundary conditions
238 induce fluxes of heat and moisture across these boundaries due to the gradient of the
239 relative field between the prescribed boundary value and that occurring inside the
240 model.

241 The above boundary conditions induces quasi-1D solutions and, for this reason, the 2D model
242 has been discretised by a structured mesh of three-nodes triangular elements, see figure 1, with
243 5 elements only through the width. The mesh has been refined close to the upper and lower
244 boundaries where high spatial gradients are expected. After a convergence study and as a
245 compromise between the conflicting requirement of accuracy and reduction of computing time,
246 finite element discretizations with 300 elements and 213 nodes and 600 elements with 423
247 nodes, were adopted for the models 120 mm and 240 mm thick, respectively.

248 The results, in terms of humidity profiles, have been calculated for a period of 10 years and
249 plotted in Figure 2 at different time increments. Two thicknesses have been considered for the
250 concrete component, i.e. 120 mm (Figures 2a,b) and 240 mm (Figures 2c,d). Two external
251 relative humidities (RHs) have adopted in the simulations and consist of 80% (Figures 2a,c)
252 and 40% (Figures 2b,d). The material parameters used in the humidity predictions have been
253 based on the mean values of ranges included in Table 2 and values specified in Table 3.

254 The results of Figure 2 highlight the ability of this model to simulate the highly non-linear
255 humidity profiles that can develop through the thickness of a typical concrete component and
256 how these can be influenced by the drying mechanism activated by the different external

257 environmental conditions and due to the selection of different section heights and wet curing
258 periods (results presented in Figure 2 have been calculated based on a wet curing period of 10
259 days). Figure 2a shows that, when exposed to a high relative humidity environment (i.e.
260 environmental RH of 80%), a thin concrete component can approach an equilibrium condition
261 of the entire cross-section with the ambient conditions after nearly a year from casting. This
262 process is slower for a thicker concrete component as highlighted in Figure 2c with thickness
263 of 240 mm in which, only after 10 years, equilibrium of the entire cross-section with the
264 environment is achieved. When considering concrete components exposed to dry environments
265 (with RH of 40%), steep humidity gradients occur in the 120 mm and 240 mm thick
266 components and, even after 10 years, equilibrium of the entire cross-section is not obtained, as
267 depicted in Figures 2b, d.

268

269 Figure 1.

270

271 Figure 2.

272

273 **3. Sensitivity analysis**

274 The design of the experiments, for inverse analysis purposes, can be improved by sensitivity
275 analysis, which is intended to compute the influence of each sought parameter on the
276 measurable quantities. The sensitivity analysis described in this section is used to gain a better
277 understanding on how the sought material parameters, i.e. those listed in the lower part of
278 Table 1, influence the variations of the relative humidity and temperature over time. In
279 particular, the sensitivity analysis is applied to enhance the selection of the most effective time
280 duration and spatial positions for the relative humidity and temperature measurements that will

281 be considered and evaluated in the implementation of the inverse analysis technique in the
282 following section, (see e.g., [23], [16]).

283 Sensitivity indices are computed as partial derivatives of relative humidity h and temperature T
284 with respect to the model parameters p_i at a certain instant in time t (taking $t = 0$ the time of
285 concrete casting) in a certain position z within the thickness of the concrete component as
286 follows:

$$S_{h,p_i}(z,t,\mathbf{p}) = \frac{\partial h(\mathbf{p},z,t)}{\partial p_i} \frac{p_i}{h(\mathbf{p},z,t)} \quad (17a)$$

$$S_{T,p_i}(z,t,\mathbf{p}) = \frac{\partial T(\mathbf{p},z,t)}{\partial p_i} \frac{p_i}{T(\mathbf{p},z,t)} \quad (17b)$$

287 These indices are normalised, for comparison purposes, with respect to the parameter value and
288 to the current and local value of the corresponding field. In the numerical computations, after
289 some preliminary convergence studies, the (first-order) derivatives have been approximated by
290 forward finite-differences with 0.1% increments, and have been evaluated in a number of
291 locations through the thickness of the concrete component and for a certain number of time
292 instants.

293 Figure 3 presents the sensitivity of the humidity profiles with respect to all model parameters
294 through the thickness of the concrete component and at representative instants in time. These
295 results have been obtained by assigning to the model parameters the mean values of Table 2
296 and those specified in Table 3, and by considering a 120 mm thick concrete component
297 exposed on its top and bottom surfaces while applying a constant external temperature of 20°C
298 and a relative humidity of 80%.

299

300

Figure 3.

301

302 The null sensitivity for all the parameters at the upper and lower sides of the model is due to
303 the Dirichlet boundary conditions assumed. The curves plotted in Figure 3 highlight how the
304 influence of the different model parameters on the relative humidity distributions varies in time
305 and space. The time instants considered in the graphs of Figure 3 have been selected to outline
306 both increasing and decreasing trends in the calculated sensitivity indices $S_{h,p_i}(z,t,\mathbf{p})$. In
307 particular, it is possible to observe that there are two regions which present the highest
308 sensitivities, with respect to all parameters, namely the mid-height of the concrete component
309 and the position about 10 mm from the external surfaces. Among the plotted parameters
310 governing moisture diffusion, the one which most affects the results in terms of humidity
311 distribution is the exponent n , characterized by a sensitivity index ten times greater than the
312 ones computed for parameters D_0 and D_1 . It is interesting to observe that the sensitivity with
313 respect to D_1 , which represent the moisture diffusion at saturation ($h = 1$), reaches its peak
314 value after 20 days and then it decreases with decreases in the humidity content. On the
315 contrary, the sensitivity with respect to D_0 , which represents the moisture diffusion at $h = 0$,
316 keeps increasing for the first 180 days while the position of maximum sensitivity moves
317 towards the mid-height of the concrete component as the desiccation process progresses.

318 Sensitivity with respect to $\mathcal{Q}_c\%$ is almost null since this parameter is expected to influence
319 primarily the variation of the temperature field. Figure 4 depicts the sensitivity indices of the
320 temperature profiles $S_{T,p_i}(z,t,\mathbf{p})$ computed only with respect to the parameters affecting this
321 field, through the thickness of the concrete component and at selected time instants based on
322 the concrete specimen and external environmental conditions described for $S_{h,p_i}(z,t,\mathbf{p})$.

323

324

Figure 4.

325

326 Figure 4 shows that the influence of the different model parameters on the temperature
327 distribution is continuously varying in time and space. In particular, it is possible to observe
328 that the region which presents the highest sensitivities, with respect to all parameters, is the
329 mid-height of the concrete component. Another important conclusion which can be drawn from
330 Figure 4 is that the highest sensitivity is achieved in the first few hours of the cement hydration
331 chemical reaction, even if the time duration of the temperature variation phenomenon is about
332 2 days.

333 When considering the time variability of sensitivity indices for the humidity field (Figure 3), it
334 is interesting to observe that the curves related to those parameters, which directly influence
335 cement hydration (A_{c1} , A_{c2} , η_c and γ_c), present a first peak after the first 10-30 days and a
336 second one (of opposite sign) after about 1 year. The time dependence associated with the
337 sensitivity indexes is illustrated in Figure 5 for a concrete component 120 mm high and for a
338 period of 10 years considering the highest $S_{h,p_i}(z,t,\mathbf{p})$ (i.e. those determined for n , g_1 , γ_c and
339 η_c). For parameters governing moisture diffusion and sorption curves (n and g_1 , respectively),
340 the maximum value for $S_{h,p_i}(z,t,\mathbf{p})$ is achieved between two and six months and after one
341 month, respectively. The other two parameters (γ_c and η_c , governing cement hydration)
342 present a maximum value after 30 days and a minimum after about one year.

343

344

Figure 5.

345

346 The trends depicted in Figure 5 for the 120 mm thick component exposed to an environmental
347 RH of 80% are slightly modified when considering a dry environment (i.e. environmental
348 RH = 40%) in Figure 6 and a larger thickness (i.e. 240 mm thick component) in Figures 7 and
349 8 with RH equal to 80% and 40%, respectively.

350

351

Figure 6.

352

353

Figure 7.

354

355

Figure 8.

356

357 In particular, Figure 6 (component with thickness of 120 mm and exposed to RH = 40%)
358 shows how the peak values of the sensitivities are postponed in time. For example, the peak
359 sensitivity for parameter n occurs after 4-5 years of casting (instead of 2-6 months observed
360 with an ambient RH of 80%), and the peak and minimum values exhibited by g_1 along the
361 different positions through the thickness take place after 1-2 months and 10-20 years,
362 respectively (instead of the single peak observed after 1 month with RH = 80%). The variations
363 for γ_c and η_c follow the trend exhibited by g_1 , with the sensitivity peak soon after the pour (at
364 about 1 month from casting) and the minimum after 2-3 years (instead of 12 months with
365 ambient RH = 80%). These results highlight how the lower environmental relative humidity of
366 40% significantly extends the transient processes associated with the moisture movements due
367 to the fact that it takes now longer time for the concrete component to find equilibrium through
368 its entire height with the surrounding environment.

369 The sensitivity indices calculated for the thicker component (i.e. 240 mm) are presented in
370 Figures 7a-d and 8a-d for ambient relative humidities of 80% and 40%, respectively. The
371 overall differences observed for the two levels of external RH are similar to those noted for the
372 120 mm thick components in Figures 5 and 6, while the larger thickness leads to longer
373 transfer processes to reach an equilibrium condition through the entire concrete component
374 and, consequently, the instants in time of the peak and minimum points are postponed.

375 Based on the numerical tests carried out on the sensitivity analysis, the implementation of the
376 inverse analysis approach presented in the following section will account for the fact that the
377 positions characterized by the highest sensitivity are the mid-height of the component and close
378 to its exposed surfaces for the humidity measurement, and just the mid-height for the
379 temperature.

380 The highest sensitivity of the temperature field occurs in the first 6 hours from casting, when
381 the humidity transport mechanism has almost not even started, as depicted by its negligible
382 sensitivity. This means that measurements of the temperature distribution in this time interval
383 are bound to enhance the identifiability of those parameters affecting this field, especially of
384 those, cement hydration depends upon.

385 **4. Inverse analysis**

386 The inverse problem is usually defined as the minimization of a suitable norm, expressing the
387 discrepancy between the experimental results and the numerical counterparts, computed as a
388 function of the sought parameters.

389 The identifiability of the different parameters contained in the hygro-thermo-chemical model
390 has been investigated following a numerical procedure well established in literature (see [24],
391 [25] and [26]) that involves the setting up and implementation of different inverse analyses that
392 start from the so-called pseudo-experimental results, i.e. results numerically generated starting
393 from a given set of model parameters and supplied in input to the inverse problem. If this is
394 well-posed, then its solution should provide in output the value of the parameters adopted to
395 generate the pseudo-experimental data.

396 The input data for the inverse problem consists of both humidity and temperature profiles taken
397 at different locations through the thickness of the concrete component and at different time
398 instants. In particular, at each instant $\tau = 1\text{K } N_{ht}$ of the time history, relative humidity $h_{e,\tau s}$ is
399 measured through the component thickness in a discretised number of locations, i.e. at

400 $s = 1K N_{hz}$. Similarly, at each instant $\tau = 1K N_{Tt}$, temperature $T_{e,\tau s}$ distribution is measured
401 along the section in a discretised number of points $s = 1K N_{Tz}$. The discretization points
402 adopted for both the space and time domains are based on the considerations obtained from the
403 sensitivity analysis that highlighted the time instants and the spatial positions where the two
404 fields are most affected by the sought parameters. Assuming to collect the model parameters to
405 be estimated (i.e. those listed in the lower part of Table 1) in vector \mathbf{p} , and denoting
406 experimental and computed quantities by subscript “e” and “c”, respectively, the discrepancy
407 between measured and computed quantities can be defined by the following norm:

$$w(\mathbf{p}) = \phi_h \sum_{\tau} \sum_s \left[\frac{1}{h_{e,\tau s}^2} (h_{n,\tau s}(\mathbf{p}) - h_{e,\tau s})^2 \right] + \phi_T \sum_t \sum_s \left[\frac{1}{T_{e,\tau s}^2} (T_{n,\tau s}(\mathbf{p}) - T_{e,\tau s})^2 \right] \quad (18)$$

408 where $\phi_h = 1/(N_{ht} N_{hz})$ and $\phi_T = 1/(N_{Tt} N_{Tz})$ are weight factors whose magnitude ensure an
409 equivalent contribution to be provided by the two terms defining the objective function.

410 The minimization of the function of Equation (19) is performed by the so-called Trust Region
411 (TR) algorithm (see, e.g. [27] and [28]). Starting from a given initialization vector, this is
412 automatically updated by means an iterative procedure based on subsequent evaluations of the
413 objective function $w(\mathbf{p})$, of its gradients and on an approximation of the hessian matrix. The
414 process stops when a priori tolerances on either the variation of the objective function or the
415 Euclidean norm of the normalized optimization variables are met.

416 A deterministic batch approach is adopted in the present investigation, which means that
417 uncertainties of both experimental measurements and system modelling are not processed
418 stochastically, but the effect of random noise of different amplitude applied to the inverse
419 problem input is considered in order to investigate the robustness of the proposed identification
420 procedure. In particular, these disturbances are generated with uniform probability density over
421 an interval centred on the exact amplitude.

422 For each adopted value of the parameters model \mathbf{p}^{ad} , the corresponding pseudo-experimental
 423 data are perturbed by different noise extractions ($n = 1 \dots N_{NOISE}$). For each noise extraction,
 424 the optimization algorithm is run several times ($i = 1 \dots N_{INIT}$) starting from different
 425 initialization vectors to avoid the solution to remain stuck in local minima that might exist
 426 given the nonlinear and non-convex nature of the objective function. The identified value, with
 427 respect to all initialization vectors, \mathbf{p}_n^{id} is computed as average of all identified values \mathbf{p}_{ni}^{id}
 428 weighted with respect to the inverse of the objective function in solution, as:

$$\mathbf{p}_{n,k}^{id} = \frac{\sum_i^{N_{INIT}} \mathbf{p}_{ni,k}^{id} \left(1/w(\mathbf{p}_{ni}^{id})\right)}{\sum_i^{N_{INIT}} \left(1/w(\mathbf{p}_{ni}^{id})\right)} \quad (19)$$

429 The error with respect to the assumed set of model parameters, for each noise extraction n , is
 430 then computed as:

$$err_{n,k}^{id} = 100 \cdot \left| \frac{\mathbf{p}_{n,k}^{id} - \mathbf{p}_k^{ad}}{\mathbf{p}_k^{ad}} \right| \quad (20)$$

431 A final error index is then computed as the average of all the single errors computed for each
 432 noise extraction as follows:

$$err_k^{id} = \frac{1}{N_{NOISE}} \sum_n^{N_{NOISE}} err_{n,k}^{id} \quad (21)$$

433 This global error norm computes the average of the absolute values of the different errors
 434 resulting from the different noise extractions to avoid compensations between errors of
 435 opposite signs when a large number of random noise extractions is adopted.

436 **4.1 Results**

437 Different inverse analysis exercises have been solved in the following to investigate the
 438 optimal formulation of the inverse problem for the identification of the parameters
 439 characterised by a large variability (i.e. those listed in the lower part of Table 1), contained in

440 the model presented in Section 2 on the basis of humidity and temperature profiles
441 measurements. In the following, only representative results are presented to outline and support
442 the key findings of this work.

443 The concrete properties adopted in the simulations are those equal to the means values of
444 Table 2 and those specified in Table 3. Drying boundary conditions have been assumed on the
445 two opposite surfaces of the concrete component (Figure 1) and the external temperature has
446 been assumed constant and equal to 296 K.

447 The first inverse analysis exercise considers a 120 mm thick concrete component exposed to an
448 environment relative humidity of 80%. In this initial simulation, no noise is added to the
449 pseudo-experimental data. Figure 9 illustrates the convergence curves of the sought parameters
450 (normalized with respect to the expected value) for two different initialization vectors.

451

452  Figure 9.

453

454 From these results, it is evident that the inverse problem is not well posed with respect to the
455 identification of parameters A_{c1} and γ_c , identified with a weighted average error of 65.5% and
456 1.8%, respectively, while all the other parameters are identified with their expected value, with
457 a maximum error of 0.2% for A_{c2} . The lack of identifiability of parameters A_{c1} and γ_c is
458 related to the form in which they appear in the hygro-thermo-chemical model when defining
459 α_c in Equation (4). This is attributed to the fact that both parameters have an equivalent effect
460 on α_c , i.e. an increase in A_{c1} leads to an increase of α_c that could be similarly produced by a
461 decrease of γ_c . Because of this behaviour, the inverse analysis procedure struggles to
462 distinguish between these two parameters. This ill-posedness of the inverse problem is

463 confirmed in Figure 10 that illustrates the variation of the objective function of Equation (18)
464 plotted with respect to A_{c1} and γ_c .

465

466 Figure 10.

467

468 From this figure, it is evident the existence of different combinations of these two parameters
469 providing the same absolute minimum of the objective function. However, due to its higher
470 sensitivity, as highlighted, for example, in Figures 3 and 4 and also by the shape of the
471 objective function in figure 10, γ_c can be still identified with a small error. The temperature T
472 located in the denominator of the exponent of the exponential function of Equation (4) (with γ_c
473 being located at the numerator of this exponent). provides only a marginal support to the
474 identification of A_{c1} and γ_c , especially when considering realistic boundary conditions that
475 enable heat exchange between the concrete component and its surrounding environment.

476 The above considerations have suggested that the following inverse analysis exercises will be
477 carried out assuming A_{c1} known a priori. This assumption is considered valid based on the fact
478 that the lack of identifiability of parameter A_{c1} previously discussed does not affect the
479 identifiability of all other model parameters, see Figure 9. The validity of this assumption is
480 later reconfirmed by the results reported in Table 6 outlining how different values for A_{c1} do
481 not influence the identifiability of the sought parameters.

482 Representative results obtained from the inverse analysis procedure are presented in the
483 following considering different arrangements for the discrete measurements of the relative
484 humidity and temperature fields together with different periods of monitoring. Different
485 concrete components and ambient conditions are used as case studies, for example varying
486 their concrete thickness, period of wet curing after casting and ambient relative humidity. All

487 pseudo-experimental results have been generated with a noise perturbation of $\pm 10\%$ to evaluate
488 the robustness of the inverse procedure. It is considered that this noise is acceptable for the
489 purpose of this study to take into account the inaccuracy and the disturbance associated with
490 the experimental measurements.

491 Table 4 reports the results obtained considering a varying number of discrete humidity
492 measurements through the thickness of the concrete component as well as the inclusion of a
493 temperature measurement. The concrete component is 120 mm thick and wet cured for 1 day
494 from casting. The ambient relative humidity is taken equal to 40% and the measurements are
495 performed for a period of 30 days (with a frequency of one measurement per hour). Column A
496 of Table 4 highlights how the use of one humidity measurement, even if selected at the mid-
497 height of the concrete component that corresponds to the point of maximum sensitivity, is not
498 sufficient for the sought parameters identification, the estimation of D_0 being affected by an
499 error (21.7%) much larger than the added noise. The use of a second relative humidity
500 measurement (located 10 mm below the exposed surface in column B of Table 4) ensures the
501 identifiability of all parameters (the observed errors are within the magnitude of the noise
502 introduced in the pseudo-experimental measurements). The inclusion of additional relative
503 humidity measurements, for example at 20 mm and 30 mm below the exposed surface, does
504 not improve the results as depicted by the values reported in columns C and D of Table 4.

505 The results outlined in columns E-G of Table 4 aim at evaluating the optimal position for the
506 second humidity measurement for a 120 mm high concrete component and show that 10 mm
507 below the exposed surface guarantees the identifiability of all parameters (column E),
508 differently from the other choices implemented that struggle in the identification of D_0
509 (columns F and G). This result is consistent with the outcomes of the sensitivity analysis that
510 shows a peak in this position (i.e. at 10 mm below the external surface) for the parameters
511 governing moisture diffusion and sorption curves.

512 The results identified in columns A-G of Table 4 have been obtained considering one discrete
513 temperature measurement located at its point of maximum sensitivity, i.e. mid-height of the
514 concrete component, therefore highlighting the adequacy of using only the selected
515 temperature measurement. The parameters identified without the inclusion of a temperature
516 measurement (reported in column H of Table 4) do not lead to a successful characterisation of
517 ϱ_c° and $A_{c,2}$. These observations highlight how the use of a temperature measurement as
518 experimental information is crucial for the identification of the model parameters ϱ_c° and $A_{c,2}$,
519 governing cement hydration, which cannot be identified if information on humidity distribution
520 only are considered.

521

522

Table 4.

523

524 The influence of varying the period used for the monitoring of the relative humidity and
525 temperature is presented in columns A-C of Table 5. For a concrete component with height of
526 120 mm, a period monitored of 30 days (column A) is sufficient for the identification of all
527 model parameters. Longer periods of 60 days (column B) and 90 days (column C) seem not to
528 improve the identifiability of the sought parameters.

529 The presence of a lower external relative humidity and, therefore, of a larger spatial gradient
530 emphasizes the moisture transport phenomena and, consequently, improve the identifiability of
531 all the parameters associated with this process. This is highlighted when comparing the results
532 of columns A (RH 40%), with D and E (RH 80%) of Table 5, where it is shown that for a
533 higher external humidity a longer monitoring period (90 days instead of 30 days) is needed to
534 identify all the sought parameters.

535 Variations in the wet curing applied after concrete casting does not seem to influence the
536 identifiability of the model parameters as, for example, depicted in columns A, F and G for wet

537 curing periods of 1, 3 and 7 days, respectively. Curing periods approaching the monitored
538 duration of the concrete component may jeopardize the identifiability of parameter D_0
539 governing moisture diffusion, as depicted in column H for a wet curing period of 14 days. Such
540 a problem could be addressed by simply modifying the period monitored for the relative
541 humidity measurements in order to gather sufficient experimental information after the end of
542 the curing period (see column I).

543

544

Table 5.

545

546 At the beginning of this section, it has been shown that the parameters A_{c1} and γ_c could not be
547 uniquely identified (Figures 9 and 10). The approach proposed in this paper to address this ill-
548 posed condition has been to assign a value to A_{c1} equal to its mean value reported in the
549 literature ($=29450 \text{ s}^{-1}$ based on the range provided in Table 2) before the application of the
550 inverse analysis procedure. The results reported in Table 6 highlight how the identifiability of
551 the model parameters is not affected when an incorrect value for A_{c1} (i.e. different from the
552 one used for the generation of the pseudo-experimental measurements) is specified in input of
553 the inverse analysis. In particular, the upper and lower limits of A_{c1} (see Table 2 for its range)
554 are used in input for the results specified in columns B and C of Table 6 (with column A
555 showing the errors determined using the exact value for A_{c1} , i.e. the value adopted to generate
556 pseudo-experimental data). These results confirm that the identifiability of all parameters is not
557 affected, except for the “companion” parameter γ_c , whose identification error increases,
558 especially when the lower limit is assumed (however always within the same order of
559 magnitude of the added noise for the cases considered).

560

Table 6.

561
562
563 The results discussed till now have been produced for a relatively thin concrete component
564 with a thickness of 120 mm. Representative errors obtained in the case of a thicker component
565 are outlined in Table 7. In this case, a longer period of measurements is needed and of at least
566 90 days (as depicted in Columns F and G) in order to let the moisture transport process develop
567 sufficiently to collect the amount of experimental information needed for the calibration of the
568 model parameters, especially of those governing moisture diffusion. Shorter monitored periods
569 (reported in columns A-C for 30 days and in columns D and E for 60 days) do not provide
570 sufficient experimental information. The use of two discrete measurements for the relative
571 humidity is still required, with one measurement taken at the mid-height of the concrete
572 component and the second one close to the exterior surfaces (errors reported in columns F and
573 G consider the location of the second humidity measurement to be carried out at 10 mm and
574 30 mm, respectively, below the exterior surface).

Table 7.

5. Conclusions

578
579 This paper considers a hygro-thermo-chemical model capable of predicting temperature and
580 moisture variations taking place over time in a concrete component and subdivides its
581 parameters into two main sets: (i) one set of parameters that can be evaluated based on the
582 concrete mix specifications or from data reported in the literature; and (ii) a second set of
583 parameters that are characterised by a large variability and, in some cases, without a precise
584 physical meaning and, therefore, not amenable to a direct measurement.

585 This paper presents a robust inverse analysis procedure for the identification of the second set
586 of parameters using temperature and relative humidity measurements as input data. The aim of
587 the present investigation is to provide an indication on the minimum (in time and space)
588 number of discrete temperature and relative humidity measurements that are required for a
589 successful identification of the sought material parameters. These results may find applications
590 in enhancing the planning of the monitoring of in-situ investigations and of experimental tests.
591 Representative results have been presented to highlight the ability of the proposed
592 methodology to identify correctly all the sought model parameters (within an error of the same
593 order of magnitude of the noise added to the pseudo-experimental data in input to the inverse
594 problem). The considerations listed below summarise the results observed for the specific case
595 studies considered in this paper associated with the identification of the concrete parameters
596 governing moisture and heat transport mechanisms:

- 597 • For the identification of the parameters governing the humidity field, at least two points
598 within the height of the concrete component have to be monitored: one at the mid-
599 height ($0.5 \times D$) and the second close to the exposed surface (preferably about 10 mm
600 below the exterior surface for the 120 mm and 240 mm thick components considered in
601 this study).
- 602 • The thicker the concrete component the larger the monitored period should be to let the
603 moisture transport process develop sufficiently in order to gather the amount of
604 experimental information needed to identify the model parameters. In the present
605 analyses, for a concrete component 120 mm thick a period of 30 days (with a frequency
606 of one measurement per hour) has been proven to be sufficient, while for a 240 mm
607 thick component at least 90 days are required.
- 608 • Information on temperature field is crucial for the identification of the parameters
609 governing the cement hydration. In the presented analyses, it has been shown that 1

610 measurement per hour taken at the mid-height of the concrete component
611 (corresponding to the position with highest sensitivity) for a period of at least 48 hours
612 from the time of casting is sufficient for the identification of the sought parameters.

613 • The presence of a lower external relative humidity emphasises the humidity transport
614 mechanism and provides a better identification of the sought parameters, especially of
615 those governing the moisture diffusion. If a larger humidity is applied (in the present
616 examples 80% instead of 40%) the monitoring period should be increased (90 days
617 instead of 30 days) in order to collect a sufficient amount of experimental information
618 needed for the present identification purposes.

619 **6. Acknowledgements**

620 The work in this article was supported under the Australian Research Council's Discovery
621 Projects funding scheme (project number DP140400529).

622

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1 Table 1. Material parameters required in input of the hygro-thermo-chemical model.

2

	Parameter	Description
Parameters calculated based on concrete mix specifications or assigned known values well accepted in the literature	c	cement content
	w/c	water-to-cement ratio
	a, b	parameters associated with the variation of the degree of cement hydration over time and taken as $a = 7.5$ and $b = 4.0$ [1]
	λ	heat conductivity
	ρ	concrete mass density
	c_t	concrete specific heat
	k_c	parameter associated with non-evaporable water and taken as 0.253 (as suggested in [12])
Parameters characterised by a large variability (see Table 2) – some of which do not possess a precise physical meaning (to be identified with the inverse analysis presented in Section 4)	A_{c1}, A_{c2}, η_c	parameters with no precise physical meaning associated with the variation of the degree of cement hydration over time
	γ_c	parameter calculated as the ratio of the hydration activation energy over the universal gas constant
	Q_c^0	total heat content per unit cement mass due to cement hydration
	κ_{vg}^c	parameter that governs the amount of water contained in the cement gel pores
	g_1	parameter that governs the shape of the sorption curve
	D_0, D_1, n	parameters that control the moisture permeability and depend on the specific concrete mix

3

4

5 Table 2. Range of variation for the parameters listed in the lower part of Table 1.

6

Parameter	Range of variation	Mean value
A_{c1}	3900 – 55000 [s^{-1}]	29450
A_{c2}	$10^{-6} - 5 \cdot 10^{-2}$	$2.5 \cdot 10^{-2}$
η_c	5.5 – 8.0	6.75
γ_c	3000 – 8000 [K]	5500
ϱ_c^6	400 – 550 [kJ/kg]	475000
κ_{vg}^c	0.10 – 0.26	0.18
g_1	1.20 – 2.20	1.70
D_0/c	$0.2 \cdot 10^{-14} - 7.5 \cdot 10^{-14}$ [m^2/s]	$3.85 \cdot 10^{-14}$
D_1/c	$4.8 \cdot 10^{-10} - 12 \cdot 10^{-10}$ [m^2/s]	$8.4 \cdot 10^{-10}$
n	3.0 – 4.5	3.75

7

8

9

Table 3. Parameters used in the proposed numerical simulations.

10

Parameter	Assumed value
c	400 kg/m ³
w/c	0.40
a	5.5
b	4.0
λ	2.3 W/m°C
ρ	2400 kg/m ³
c_t	1100 J/kg°C
k_c	0.253

11

12

13 Table 4. Results of the inverse analysis exercises in terms of err_k^{id} [%]: varying location of
 14 discrete measurements for the relative humidity h and the temperature T .

15

D [mm]	120							
RH	40%							
Period of wet curing	1 day							
Period monitored	30 days							
Location of discrete measurements ¹								
for h [mm]	60	60/10	60/20/10	60/30/20/10	60/10	60/20	60/30	60/10
for T [mm]	60				60			none
Column	A	B	C	D	E	F	G	H
D_0	21.7	5.9	4.5	5.2	5.9	11.9	14.7	6.3
D_1	3.1	3.9	2.9	4.8	3.9	2.9	3.1	7.2
n	3.3	0.7	0.6	1.0	0.7	1.7	2.5	0.8
κ_{vg}^c	7.1	2.5	2.0	2.2	2.5	3.1	7.3	7.2
g_l	5.4	3.7	3.6	4.7	3.7	5.3	4.1	6.6
γ_c	0.1	0.3	0.2	0.2	0.3	0.2	0.1	1.5
$\varrho_c^{\%}$	4.4	2.4	1.8	3.5	2.4	4.2	2.2	11.1
A_{c2}	6.5	5.6	5.4	4.7	5.6	6.3	5.9	37.8
η_c	6.2	3.1	3.2	4.4	3.1	5.1	4.5	5.5

16 NOTE: ¹Locations measured from external surfaces of concrete component [mm].

17

18 Table 5. Results of the inverse analysis exercises in terms of err_k^{id} [%]: varying the period
 19 monitored, the external relative humidity RH and the period of wet curing after casting.
 20

D [mm]	120								
Location of discrete measurements for h [mm] ¹	60/10								
Location of discrete measurements for T [mm] ¹	60								
Period monitored [days]	30	60	90	30	90	30			14+29 ²
RH	40%			80%	80%	40%			40%
Period of wet curing [days]	1			1	1	3	7	14	14
Column	A	B	C	D	E	F	G	H	I
D_0	5.9	3.3	4.4	10.3	8.7	7.1	7.9	13.3	5.0
D_1	3.9	3.0	2.4	3.6	3.3	2.8	2.5	2.5	3.9
n	0.7	0.5	0.6	1.2	0.8	1.0	1.2	2.0	0.7
κ_{vg}^c	2.5	1.9	2.4	4.0	5.0	2.4	2.6	2.8	1.7
g_l	3.7	4.1	2.5	4.9	4.3	2.6	3.7	2.4	5.0
γ_c	0.3	0.2	0.2	0.1	0.1	0.1	0.1	0.1	0.1
\mathcal{Q}_c^{δ}	2.4	2.8	1.6	3.0	2.0	2.7	3.1	1.7	3.8
A_{c2}	5.6	5.4	4.0	3.2	4.4	4.4	5.2	5.1	4.1
η_c	3.1	3.5	1.8	3.7	2.7	2.4	4.4	2.8	5.2

21 NOTE: ¹Locations measured from external surfaces of concrete component [mm].
 22 ²Period monitored for the relative humidity measurements after the completion of the
 23 wet curing period.
 24

25 Table 6. Results of the inverse analysis exercises in terms of err_k^{id} [%]: varying the period
 26 monitored, the external relative humidity RH and the period of wet curing after casting.

27

D [mm]	120		
RH	40%		
Period of wet curing	1 day		
Period monitored	30 days		
Location of discrete measurements for h [mm] ¹	60/10		
Location of discrete measurements for T [mm] ¹	60		
Parameter A_{c1} [s^{-1}]	29450	3900	55000
Column	A	B	C
D_0	5.9	6.0	6.4
D_1	3.9	4.5	4.1
n	0.7	0.7	0.7
κ_{vg}^c	2.5	3.2	2.6
g_l	3.7	4.7	3.7
γ_c	0.3	10.8	2.9
$\mathcal{Q}_c^{\%}$	2.4	2.8	2.3
A_{c2}	5.6	5.2	5.0
η_c	3.1	3.4	2.7

28 NOTE: ¹Locations measured from external surfaces of concrete component [mm].

29

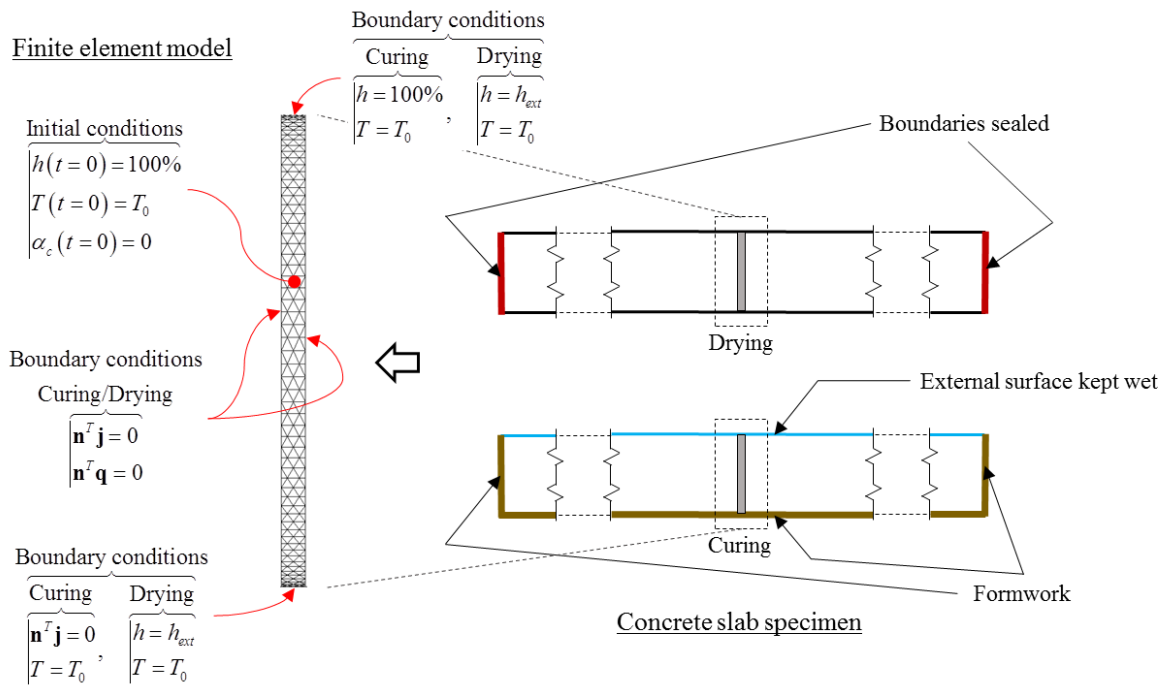
30 Table 7. Results of the inverse analysis exercises in terms of err_k^{id} [%]: varying the period
 31 monitored and the location of the discrete measurements for the relative humidity for a thicker
 32 concrete component.

33

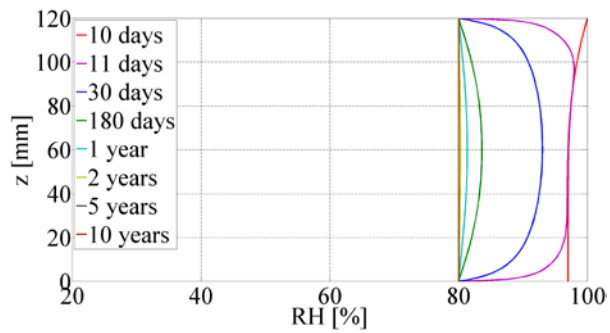
D [mm]	240						
RH	40%						
Period of wet curing	1 day						
Location of discrete measurements for T [mm] ¹	120						
Period monitored [days]	30			60		90	
Location of discrete measurements for h [mm] ¹	120/10	120/20	120/30	120/10	120/30	120/10	120/30
Column	A	B	C	D	E	F	G
D_0	7.8	16.2	27.9	5.0	7.0	3.3	6.1
D_1	6.7	5.1	4.9	5.7	5.4	3.4	3.2
n	1.1	3.1	3.2	0.8	1.0	0.6	0.9
κ_{vg}^c	5.1	6.6	9.7	5.6	10.6	5.7	5.8
g_l	6.7	8.5	8.8	5.1	8.1	4.1	3.7
γ_c	0.5	0.4	0.3	0.4	0.5	0.2	0.2
$\varrho_c^{\%}$	2.8	4.9	3.4	1.5	2.1	1.5	1.1
A_{c2}	13.4	10.1	10.1	11.5	14.1	6.4	6.4
η_c	5.7	7.6	6.2	4.0	5.4	2.3	2.3

34 NOTE: ¹Locations measured from external surfaces of concrete component [mm].

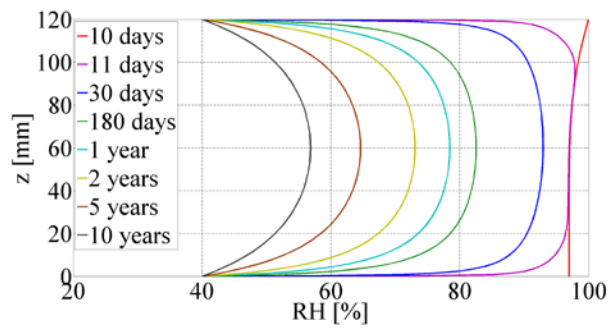
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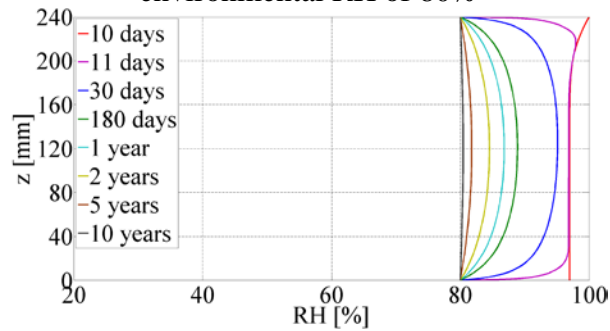
1
 2 Figure 1. Typical concrete component used in the simulations: finite element model, initial and
 3 boundary conditions.
 4



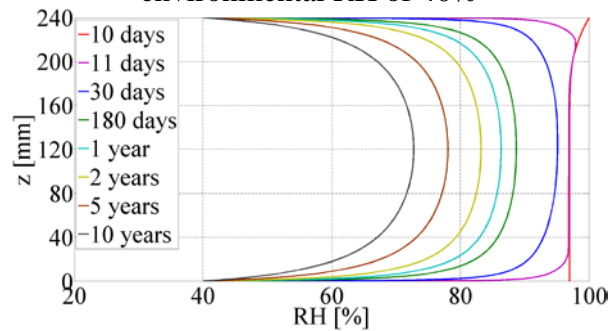
(a) concrete thickness of 120 mm and environmental RH of 80%



(b) concrete thickness of 120 mm and environmental RH of 40%



(c) concrete thickness of 240 mm and environmental RH of 80%



(d) concrete thickness of 240 mm and environmental RH of 40%

5

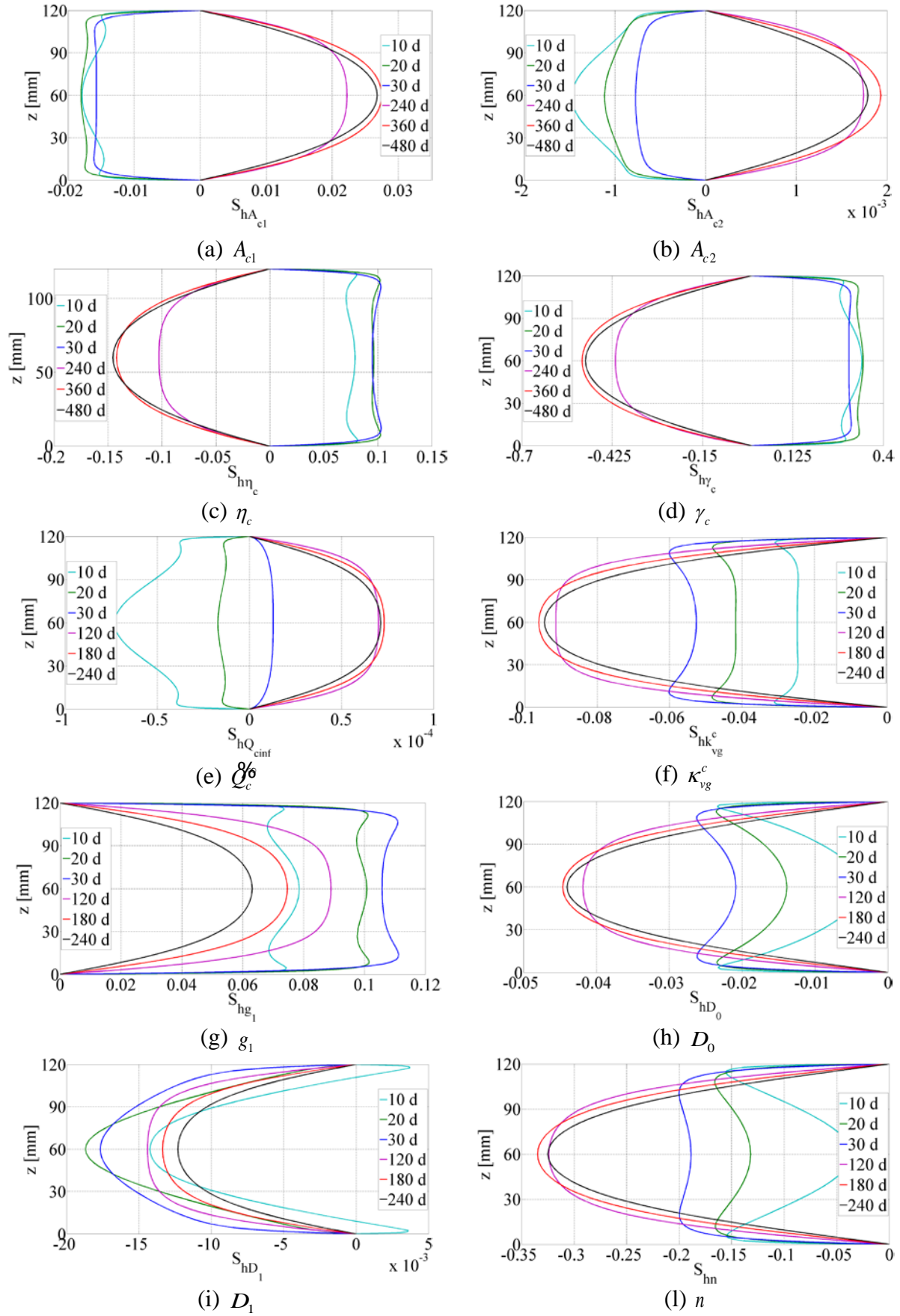
6

Figure 2. Humidity profiles for 10 years of simulation

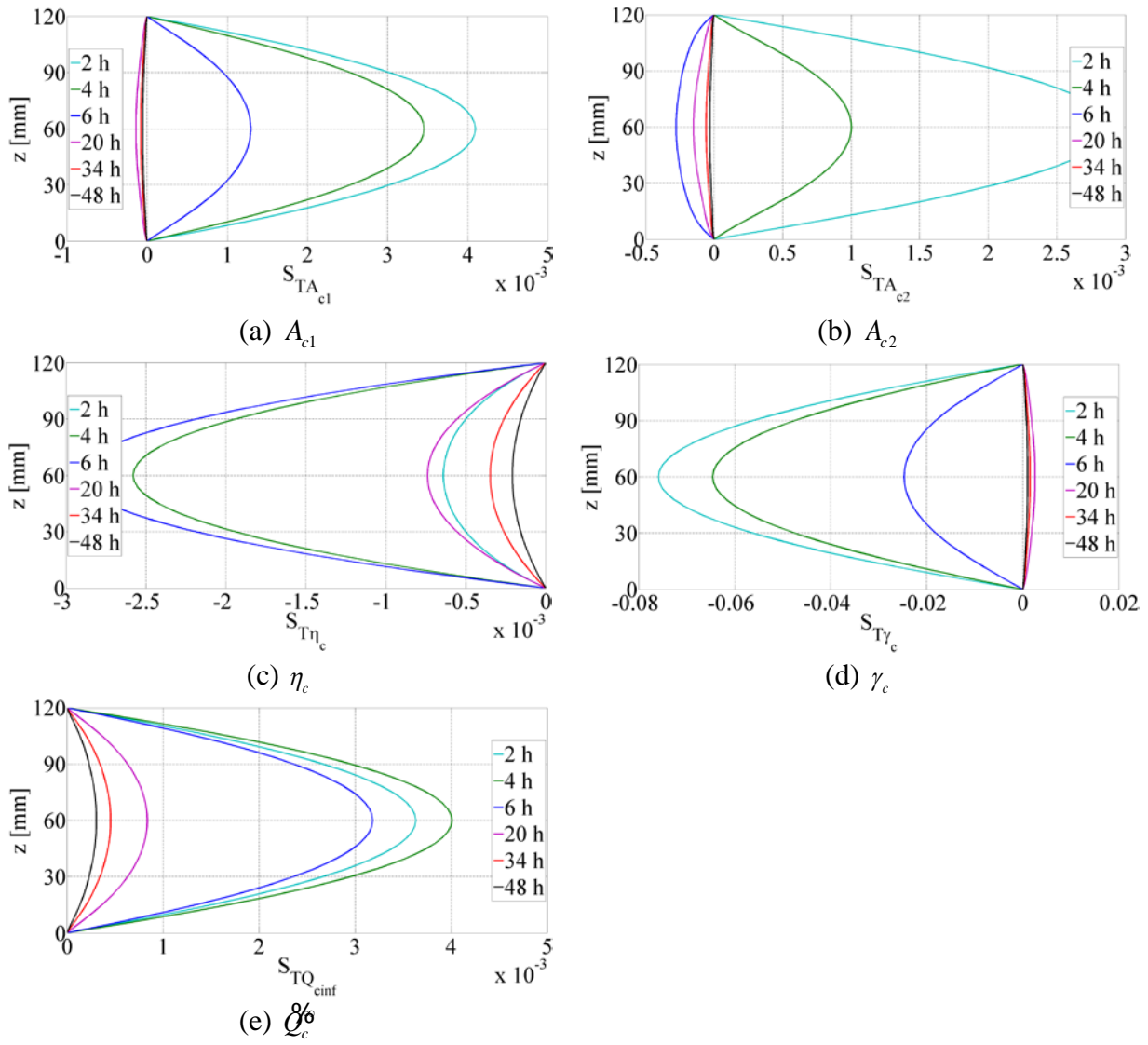
7

for typical concrete components (Figure 1) with thicknesses of 120 mm and 240 mm.

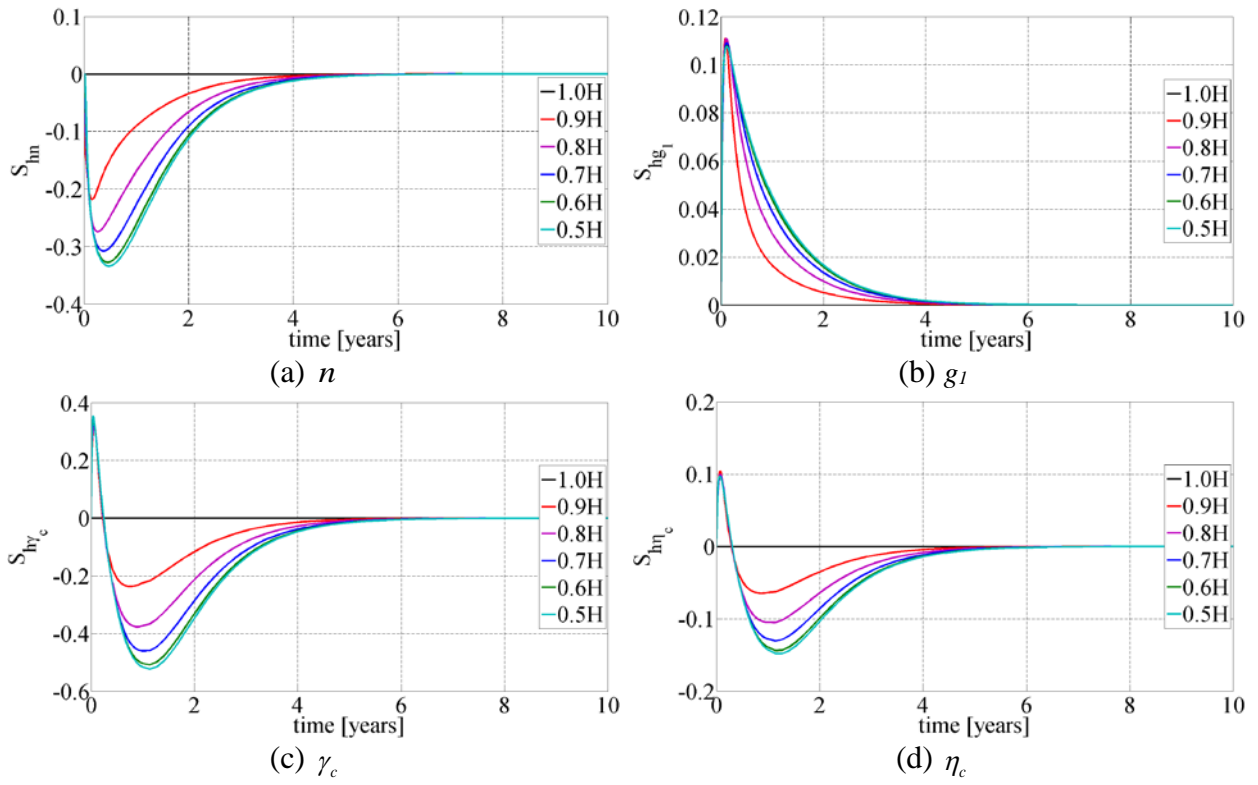
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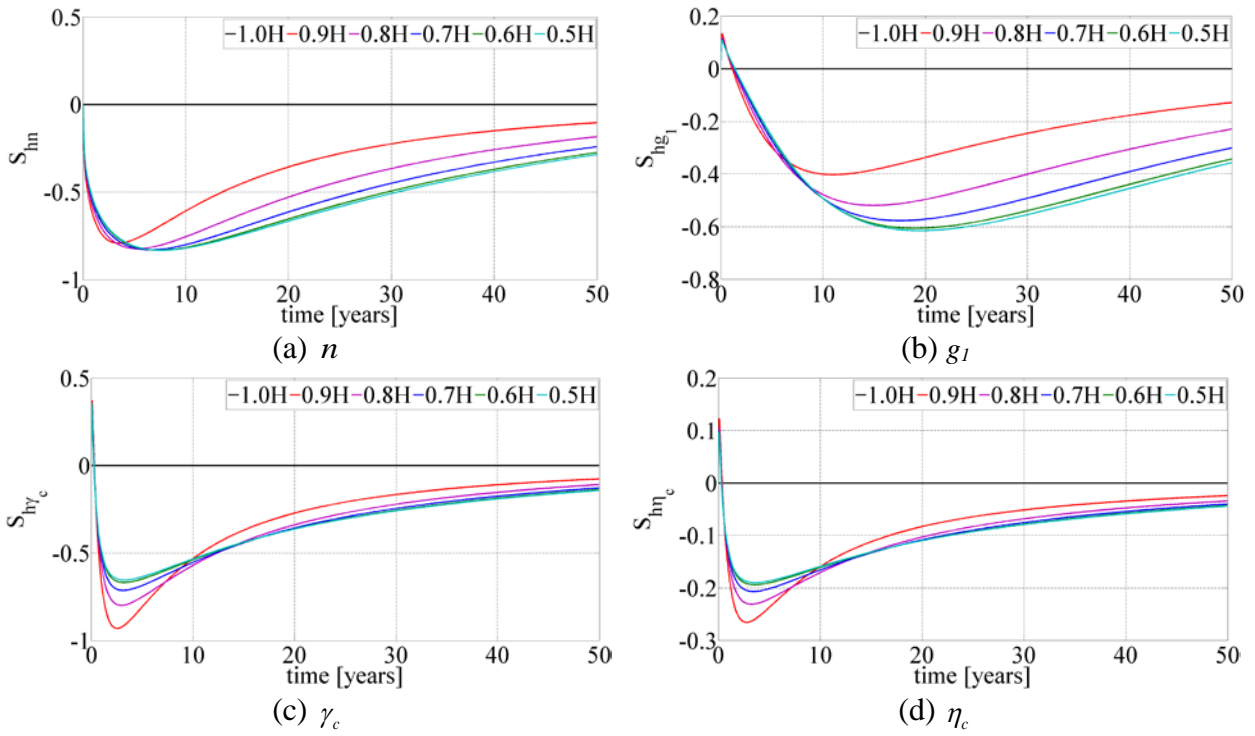
9 Figure 3. Sensitivity of humidity profiles with respect to the different model parameters.



10
 11 Figure 4. Sensitivity of temperature profiles with respect to the selected model parameters.
 12

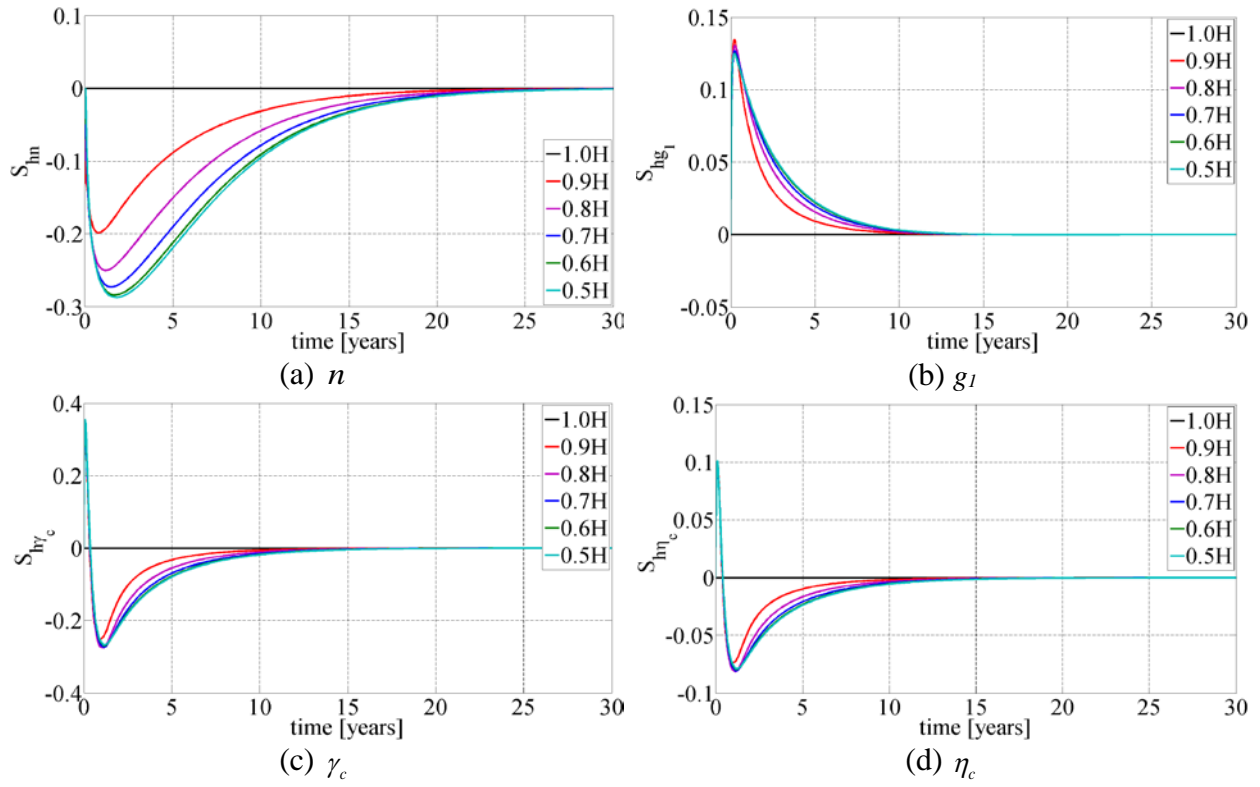


13
 14 Figure 5. Time dependence of the maximum sensitivity indices at selected locations through the
 15 concrete component height H of 120 mm exposed to an ambient RH of 80%.



16
 17 Figure 6. Time dependence of the maximum sensitivity indices at selected locations through the
 18 concrete component height H of 120 mm exposed to an ambient RH of 40%.

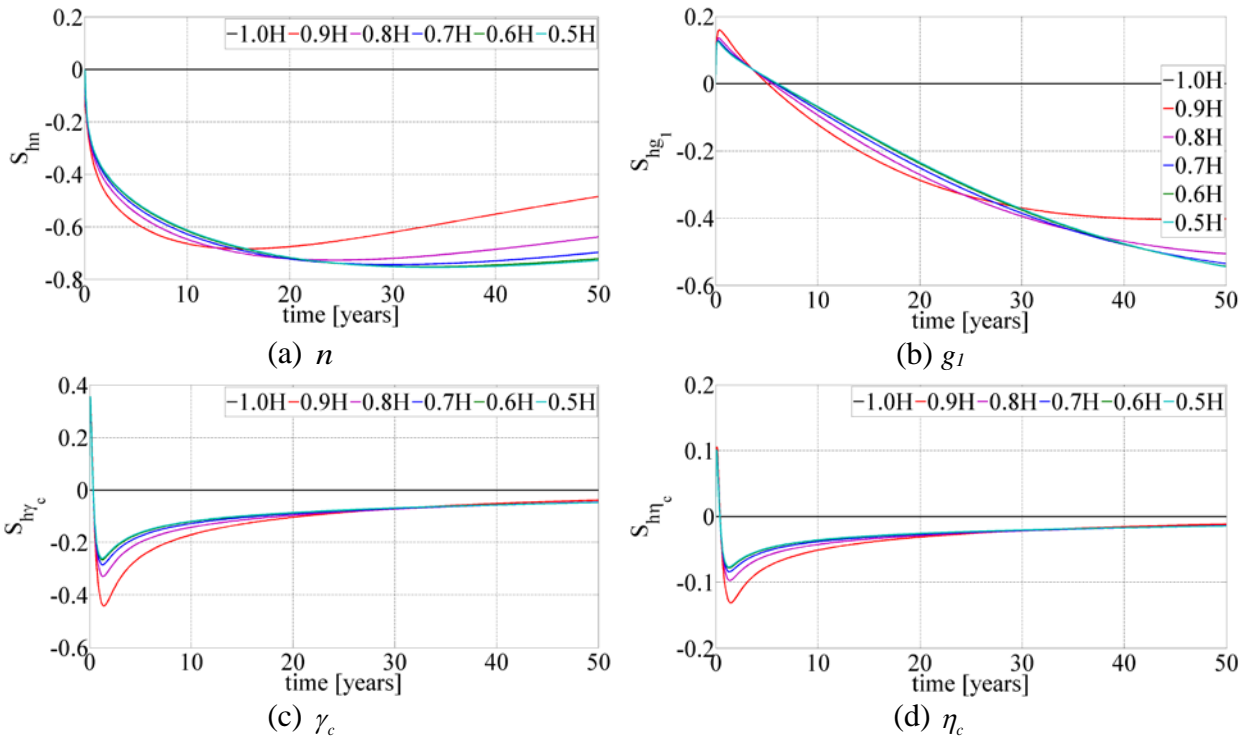
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20

21 Figure 7. Time dependence of the maximum sensitivity indices at selected locations through the

22 concrete component height H of 240 mm exposed to an ambient RH of 80%.

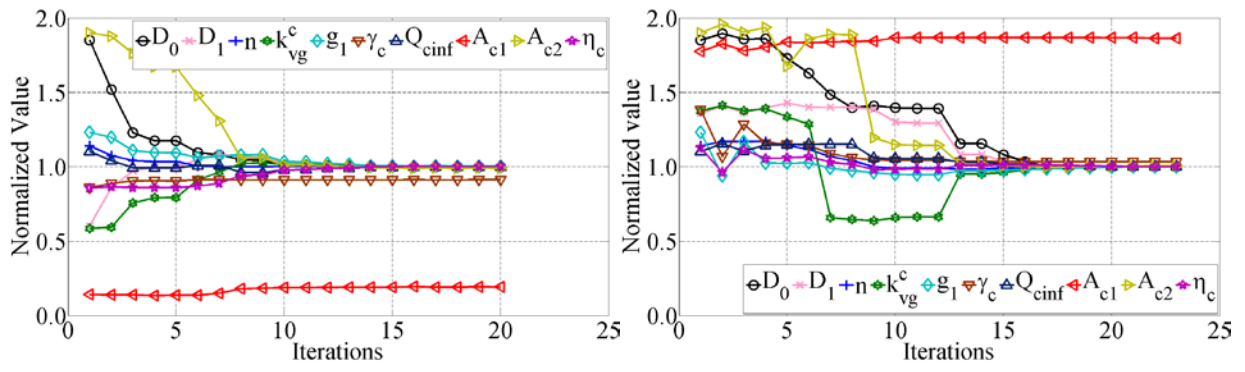


23

24 Figure 8. Time dependence of the maximum sensitivity indices at selected locations through the

25 thickness of the 240 mm concrete component exposed to an ambient RH of 40%.

26

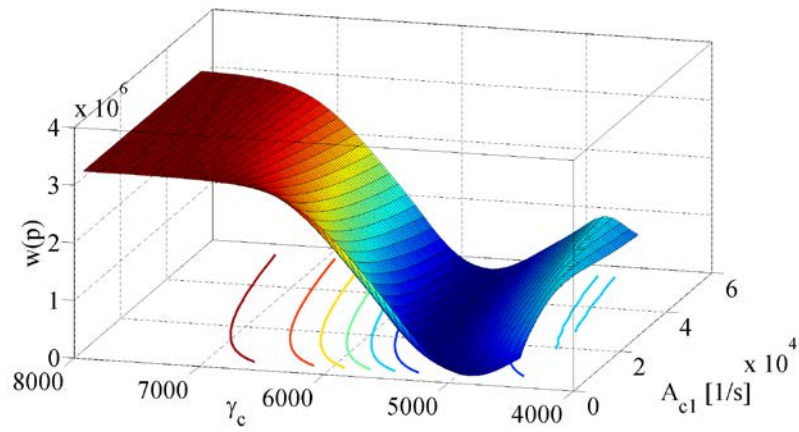


27

28

29 Figure 9. Convergence curves of the sought parameters (normalized with respect to the expected
 30 value) for two different initialization vectors.

31



32

33

34

Figure 10. Objective function in equation (19), plotted with respect to A_{cl} and γ_c .

35