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# Blind comparison of saturation ratio profiles on large RC structures by means of NDT and SFE - Application to the VeRCoRS mock-up

Ritesh Gupta<sup>a</sup>, Donatien Rossat<sup>a,b</sup>, Xavier Dérobert<sup>c</sup>, Julien Baroth<sup>a,\*</sup>,  
Matthieu Briffaut<sup>d</sup>, Géraldine Villain<sup>c</sup>, Frédéric Dufour<sup>a</sup>

<sup>a</sup>*Univ. Grenoble Alpes, CNRS, Grenoble INP, 3SR, 38000 Grenoble, France*

<sup>b</sup>*Electricité de France (EDF-DIPNN-DT), 69007 Lyon, France*

<sup>c</sup>*Univ Gustave Eiffel, Campus de Nantes, F-44344 Bouguenais, France*

<sup>d</sup>*Univ. Lille, CNRS, Centrale Lille, UMR 9013 - LaMcube - Laboratoire de Mécanique, Multiphysique, Multiéchelle, F-59000 Lille, France*

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## Abstract

The prediction of large concrete structures behaviour such as bridges, dams and nuclear containment buildings (NCB) is a vital issue regarding the evaluation of the durability, safety and effect on the surrounding environment. In this work, experimental and numerical estimations of the saturation ratio profiles in the VeRCoRs NCB mock-up structure are presented, and their blind comparison is discussed. Non-destructive testing (NDT) based capacitive measurements are processed to quantify the saturation ratio experimentally. Then, a weakly coupled thermo-hydric (TH) finite element model is presented within the serviceability state of VeRCoRs for the numerical counterpart. The uncertainty in the capacitive measurements and the constitutive parameters of the numerical model are highlighted as coming from the following three sources: (a) the natural randomness of the material properties and physical processes, (b) the limited

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\*Corresponding author

Email address: [julien.baroth@3sr-grenoble.fr](mailto:julien.baroth@3sr-grenoble.fr) (Julien Baroth)

knowledge of some input parameters in the mathematical model either obtained experimentally at the specimen scale and (c) empirically derived in the exploitation of the physical process. The influence of the uncertainty in the saturation ratio estimations is presented by error bars experimentally and is addressed by a stochastic finite element (SFE) study in the numerical work. Accounting for uncertainties in NDT and SFE measurements, the mean values of saturation ratio (reported in %) profile are forecasted up to 40% and 34% respectively, with standard deviation for both in the range of 3.5-4.5% in magnitude.

*Keywords:* Concrete structures, Saturation ratio, Spatial distribution, Non-destructive capacitive measurements, Stochastic finite element analysis, Uncertainty quantification

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## 1. Introduction

The prediction of the fluid-tightness of large concrete structures, especially those with a containment role such as Nuclear Containment Buildings (NCB), plays a crucial role in their serviceability and longevity and, most importantly, the safety of the surrounding environment. These large containment structures undergo complex physical processes (*e.g.*, concrete ageing) over their lifespan, and thus, the tightness evolves significantly during the lifetime of the structure. Therefore, it is necessary to account for uncertainties associated with numerical forecasts to quantify structural integrity and tightness risks and, therefore, provide decision aids for improving their maintenance. Apart from cracking at an early age at the outer structure surfaces, which is out of the scope of our contribution, concrete drying, a key durability indicator, must be carefully ad-

13 dressed. Concrete drying is a vital issue for the air-tightness of the structure  
14 as more connected porosity becomes available for gas molecule transfer upon  
15 drying. Besides, drying is of great importance for prestressed structures since  
16 the drying induced shrinkage accelerates the loss of prestressing effects.

17 To these ends, the VeRCoRs NCB mock-up has been chosen as an appli-  
18 cation case of a containment building in this work [1]. VeRCoRs is a 1 : 3  
19 structural scale mock-up of the double-wall containment enclosure constructed  
20 by EDF to experimentally analyse the time evolution of properties and be-  
21 haviour of the containment enclosures under actual operating conditions. VeR-  
22 CoRs (*Vérification Réaliste du Confinement des Réacteurs*) is a French acronym  
23 meaning ‘realistic verification of the containment of the reactors’. The concrete  
24 drying behaviour investigation is taken as a proxy to address the aforementioned  
25 critical issues. The evolution of the saturation ratio is considered representative  
26 of the drying behaviour.

27 When considering the assessment of concrete structures on-site, non-destructive  
28 testing (NDT) techniques enable to completion of visual inspections and provide  
29 means to improve the reliability in the evaluation. Several NDTs have been de-  
30 veloped for civil engineering applications, as being sensitive to different material  
31 properties like durability indicators and state parameters. Ultrasonic methods  
32 are applied for strength assessment through elastic modulus measurement and  
33 defect detection like the presence of air and crack [2, 3]. Also, the electromag-  
34 netic (EM) methods are proven sensitive to the water and ionic content [4, 5].  
35 Therefore, they are helpful to measure the dielectric permittivity and electric

36 resistivity in concretes.

37 In recent years, non-destructive measurements have notably been provided  
38 by the ENDE (*Evaluation Non Destructive des Enceintes de confinement des*  
39 *centrales nucléaires*) research project, thanks to the PIA-RNSR French National  
40 Program, involving a wide range of non-destructive measurement techniques  
41 of several concrete properties (Young's modulus, porosity, permeability). The  
42 significant amount of measurement points provided by such techniques enables  
43 to perform much more consistent statistical inference.

44 The capacitive measurements are part of non-destructive testing (NDT)  
45 techniques useful for the evaluation of concrete structures [6, 7]. NDT tech-  
46 niques are not only significant for detecting peculiarities but also helpful in  
47 assessing concrete material properties and their spatial distribution and time  
48 evolution, like saturation ratio, during the diagnosis of civil engineering struc-  
49 tures [5]. However, auscultation cannot only be based on NDTs as each one can  
50 be related to more than one durability indicator (*e.g.* saturation ratio, poros-  
51 ity and compressive strength). Hence, destructive tests (DT) are necessary to  
52 confirm and calibrate the results obtained by NDT auscultation [8].

53 Besides, numerical models are used to assess the pertinence of in-situ mea-  
54 surements and also predict the long term effect of ageing on the future be-  
55 haviour of concrete [9]. Several numerical studies have been performed to assess  
56 the physical processes linked to large concrete containment structures in recent  
57 years. Several numerical models are available for purpose of covering the ther-  
58 mal [10] and hydric [11, 12, 13, 14] behavior of concrete using either a fully

59 coupled approaches [15, 16, 17, 18, 19] or chained calculation strategies [20, 21]  
60 also called weakly-coupled approaches. Based on our past experience [9, 22] and  
61 the results of the international blind benchmark [1], a weakly-coupled approach  
62 is chosen to offer an efficient optimum in this contribution. Thereby, drying is  
63 the only aging phenomenon taken into account in the present work. Notably,  
64 the hydric behaviour in this work refers to the time evolution of the moisture in  
65 the concrete and therefore can be interchangeably referred to as the hydraulic  
66 behaviour, a representative of the moisture transfer phenomenon.

67 In general, the model accuracy is dependent on the boundary conditions  
68 (BCs) and the uncertainties related to the concrete's properties' identification.  
69 These modelling approaches present the detailed deterministic description of  
70 the associated physical processes, accounting for the uncertainty in the input  
71 parameters and the uncertainty of the numerical forecast. For this, the general  
72 uncertainty Quantification (UQ) framework enables one to account for uncer-  
73 tainties associated with material properties, loads, or boundary conditions and  
74 quantify their influence on numerical predictions. It is generally achieved by us-  
75 ing elements of probability theory, by modelling input parameters of a physical  
76 model as random variables and estimating statistical moments or probability  
77 density functions (PDFs) of the model response. In addition, simulation meth-  
78 ods such as Monte-Carlo (MC) combined with surrogate modelling techniques  
79 are often used in this context [22]. The stochastic finite element (SFE) model  
80 forecast incorporates the law of large numbers and the central limit theorem to  
81 quantify the model response converging towards a mean magnitude.

82 In this work, independent experimental and numerical works towards esti-  
83 mating the saturation ratio profile in the VeRCoRs mock-up are presented and  
84 blindly compared. The capacitive measurements provide an extensive data set  
85 for the in-situ experimental measurements. A sparse Polynomial Chaos Expan-  
86 sion (PCE) surrogate of the thermo-hydric (TH) numerical model represents  
87 the stochastic saturation ratio.

88 The outline of the present work is briefed hereafter. First, the problem  
89 statement in the context of the VeRCoRs mock-up is presented. Second, the  
90 experimental work comprising the EM characterisation of the constituent con-  
91 crete on the lab-scale specimens towards the calibration of the saturation ratio  
92 and in-situ capacitive measurements and their post-processing for the satura-  
93 tion ratio estimation is presented. Third, a numerical work comprising the finite  
94 element model representative of the VeRCoRs mock-up for a deterministic and  
95 stochastic estimation of the saturation ratio is presented. Lastly, the blind com-  
96 parison of the saturation ratios estimations from two independent campaigns is  
97 presented alongside a discussion on agreement and difference.

## 98 **2. Problem statement**

99 This section presents the structural layout of the VeRCoRs mock-up, the  
100 concrete mix design composition and pressurization test loading history consid-  
101 ered in this work. VeRCoRS is a non-nuclear containment mock-up; however,  
102 it is subjected to the same operating conditions as those familiar to a nuclear  
103 containment building. In addition, the mock-up is highly instrumented (*e.g.*

104 more than 700 sensors, 2 km of optical fibre and pendulums), providing real-  
 105 time access to a database of physical measurements covering its entire operating  
 106 life [1]. The concrete mix design of the VeRCoRs mockup enclosure is presented  
 107 in Table 1.

Table 1: Concrete mix design of VeRCoRs mock-up, from [1]

Component		Quantity	Unit
Cement	CEM I 52.5	320	$kg/m^3$
Water		197.6	$l/m^3$
Sand	0/4 (GSM LGP1)	830	$kg/m^3$
Gravel	4/11 (GSM LGP1)	445	$kg/m^3$
	8/16 (Balloy, Seine-et-Marne)	550	$kg/m^3$
Admixture	Plasticising adjuvant	2.4	$l/m^3$
Density		2386	$kg/m^3$
w/c ratio	by weight	0.62	

108 Due to its reduced scale, the model ages more quickly than an actual en-  
 109 closure. According to the preliminary studies of the project, a factor of 9 is  
 110 retained to exploit the drying kinetics [1]. So a 60-year operating life for an  
 111 actual enclosure would be represented by only 6.5 years at the 1:3 scale model.  
 112 It allows simulating accelerated yet realistic drying behaviour during 60 years  
 113 of operation.

114 The containment structure is made up of different structural components

115 of different dimensions and varying thicknesses, presented in Figure 1. Dimen-  
 116 sional differences cause heterogeneous ageing in the structure as thin elements  
 117 tend to age faster than thick elements. Moreover, it gives rise to differential  
 118 deformations exposing the relatively thinner parts to a greater risk of cracking.  
 119 Thus, wall region of 14.68m height, as seen from Figure 1b, is the focused area  
 120 in the present work for the estimations of the saturation ratio profiles experi-  
 121 mentally and numerically.

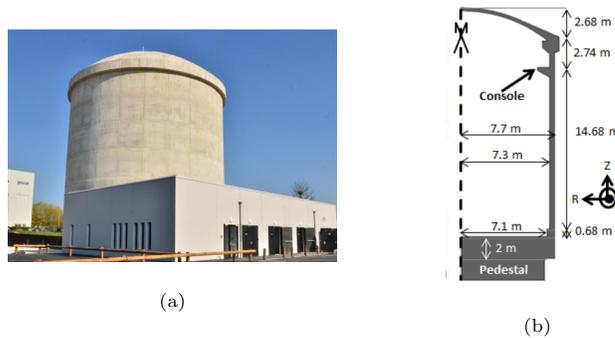


Figure 1: General overview of the VeRCoRs mock-up, presenting (a) isometric view [23] (b) an asymmetric vertical sector of the inner wall of the mock-up, from [9]

122 A sequence of standardized pressurization tests verifies the serviceability  
 123 of a full-scale NCB. First, tests are performed after prestressing the contain-  
 124 ment building and the commissioning of the reactor, named as pre-operational  
 125 visit (VPO - *Visite pré-opérationnelle*). Next, the following test is performed  
 126 three years after the first fuel loading named as additional visit (VC - *vis-  
 127 ite complémentaire*). Then every ten years, ten-yearly visits (VD - *visites  
 128 décennales*). The scaled-down test timeline for the VeRCoRs mock-up is pre-  
 129 sented in Figure 2.

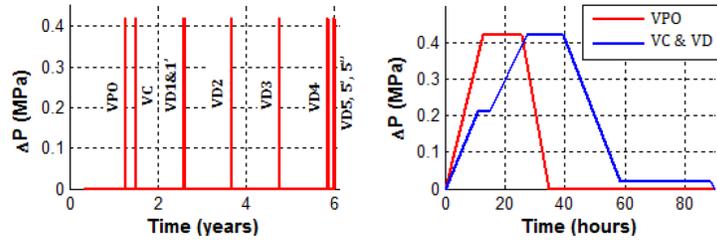


Figure 2: Pressurization/depressurisation tests timeline in VeRCoRs mock-up, from [9]

130 The pressure rise profiles differ from one enclosure to another; however, the  
 131 principle remains the same [24, 25]. A gradual increase in the internal pressure  
 132 until the target value of 5.2 bars absolute pressure is reached. The level is  
 133 maintained at this sizing pressure for 24 hours, then progressive reduction of the  
 134 overpressure until return to atmospheric pressure. The tests on the VeRCoRs  
 135 mock-up enclosure are carried out under less aggressive conditions than for a full-  
 136 scale model to avoid potential damage in the structure compromised in its future  
 137 containment capacities [26]. Here, the dry air is inhibited, at a temperature of  
 138  $20^{\circ}\text{C}$ , at a similar pressure difference between the inner and outer surface of the  
 139 internal wall of 4.2 bars for the pressurization tests. In-situ NDT measurements  
 140 on the containment structure during the pressurization tests provide extensive  
 141 databases to assess its behaviour and estimate the relevant durability indicators.  
 142 In the present work, the database recorded at the time instance of the test VD3  
 143 is presented hereafter to assess the saturation ratio.

### 144 **3. Experimental saturation ratio estimation**

145 The experimental campaign in the present work comprises of two parts.  
146 First, the electromagnetic characterisation of the VeRCoRs concrete is presented  
147 to define its complex permittivity characteristics. Subsequently, a calibration  
148 campaign on lab-scale samples with a similar mix design as of a vercors mock-up  
149 is presented to establish a relationship between concrete saturation ratio and  
150 relative permittivity measurements. Second, the calibrated relationship from  
151 the first part is used to characterise the on-site relative permittivity database  
152 extracted using electrode probes in the framework of the ENDE project as the  
153 on-site saturation ratio measurements. The description of the experimental  
154 work activities is presented hereafter.

#### 155 *3.1. Electromagnetic characterization of VeRCoRs concrete*

156 The on-site capacitive technique is presented characterising the in situ di-  
157 electric media in the 30–35 MHz frequency band to measure the saturation ratio  
158 profile in different locations. A calibration methodology is necessary to evaluate  
159 the saturation ratio in various civil engineering structures [27]. Such methodol-  
160 ogy is based on the complex permittivity measurement on various dispersive con-  
161 cretes. The permittivity measurements are carried out by a cylindrical coaxial  
162 electromagnetic (EM) transition line. It allows the laboratory characterisation  
163 of the material specimens in a large ground penetration radar (GPR) frequency  
164 band (50– 1200 MHz approx.) such as asphalt or concrete mixes [28].

165 Thereby, large campaigns of EM characterisation of numerous concrete mixes

166 are processed to evaluate the influence of every composition parameter on the  
167 complex permittivity in the GPR frequency band, using a multi-linear polyno-  
168 mial model from [29]. In addition, several tests were performed studying the  
169 effect of water content, chloride content and carbonation on the complex per-  
170 mittivity of concrete mixes [30]. EM NDT is sensitive to the volumetric water  
171 content in the porous material. However, as structure engineers characterise  
172 moisture using saturation rate, EM laboratory measurements are transformed  
173 in saturation ratio values while considering the material bulk density. Therefore,  
174 in this work, the study on the saturation ratio parameter only is presented.

175 A methodology is developed to extrapolate EM cell measurements at low  
176 frequencies, using the four-parameter variant of Jonscher's model [27]. It enables  
177 to obtain dispersion curves of the complex permittivity for extensive frequency  
178 bands, including the frequency range of the capacitive technique ( $\approx 33$  MHz).

179 In the ENDE project framework, nine concrete cores, each 70 mm long  
180 and 75 mm in diameter, are extracted from the concrete block prepared with  
181 the concrete mix design and at a timeline same as in VeRCoRs mock-up VD3  
182 pressurisation test (see Figure 2). Eight cores are extracted from the center of  
183 the block and one from the surface. They are conditioned in the laboratory until  
184 the homogeneous saturation of about 100%, 70%, 50% and 10% are achieved  
185 [31]. The experimental campaign presents the macro-porosity measurements  
186 reported based on the amount of water present in the sample between dry and  
187 saturated states in normalised conditions [32].

188 The measured values of the concrete permittivities at different saturation

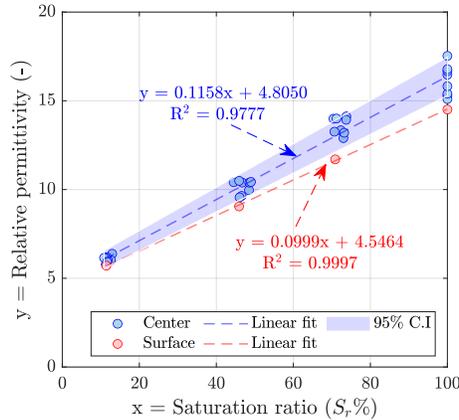


Figure 3: Permittivity (33 MHz) vs saturation ratio calibration curve for the VeRCoRs concrete

189 ratios, including a linear regression to present the overall trend, are presented  
 190 in Figure 3. The regression obtained from the surface core is assumed to be a  
 191 relatively better representative of capacitive measurements, which remain ap-  
 192 plicable to the first few centimetres of the VeRCoRs mock-up structure wall.  
 193 A standard deviation of 0.37 is reported on the permittivity measurements of  
 194 the center core is observed reported from the sample set of measurements. It  
 195 induces a default uncertainty of  $\pm 3.20\%$  on the saturation ratio magnitude ob-  
 196 tained from a permittivity value using the calibration slope of the center cores.  
 197 Besides, a porosity of 14.5% and a carbonation depth of about 3 mm is observed  
 198 from the surface core. In contrast, the porosity measured from the average of the  
 199 center cores is 15.8%. Higher relative permittivity measurements corresponding  
 200 to the center cores can be inferred due to the relatively higher porosity.

201 *3.2. Capacitive measurements on VeRCoRs mock-up*

202 This section describes the principle of capacitive measurements conducted  
203 on VeRCoRs mock-up. The aim is to estimate the saturation ratio from the  
204 capacitive measurements while discussing the various sources of uncertainty.  
205 The principle of the technique used to investigate VeRCoRs mock-up is based  
206 on the measurement of a resonant frequency (around 33 MHz) of an oscillating  
207 electric circuit RIC (resistor/inductor/capacitor) type between electrodes placed  
208 on the testing material. The set of the electrodes and the medium forms the  
209 capacitor of the RIC circuit. It is dependent on the geometry of the electrodes  
210 and the relative permittivity of the medium [5].

211 The interest of a set of various electrodes is to be able to reach varying  
212 penetration depths and thus obtain information of a gradient along with depth  
213 [33]. Various electrode probes and geometrical parameters associated with op-  
214 erating frequency facilitate variation in investigation volumes corresponding to  
215 coupling volumes. The volume of material visible by the sensor influencing the  
216 measurement is termed the coupling volume. This technique is suitable for mea-  
217 suring the saturation ratio of porous materials, such as concrete. The system  
218 designed by the Technical and Scientific Network of the French Ministry of the  
219 Ecological Transition comprises a panel of several electrodes [6]. In this work,  
220 the electrodes PE (5x70 mm), ME (10x70 mm), M3E (15x70 mm) having cou-  
221 pling volumes of thicknesses about 7, 17 and 22mm respectively are used, as  
222 presented in Figure 4.

223 A calibration step is necessary to link the resonant frequency to a permit-



Figure 4: Capacitive measurements electrodes PE, ME and M3E as seen from left to right

224 tivity value, considering the medium as homogeneous and semi-infinite. Several  
225 known materials are used as reference whose permittivities are measured in an  
226 EM cell. These materials include PVC, Teflon, marble, granite, limestone and  
227 eccostock, a rigid polyurethane foam of high permittivity [28]. Moreover, the  
228 interference effects of the external environment and the capacitive system is re-  
229 moved by a complementary measurement in the air, subtracted to the surveyed  
230 medium measurement. Thus, the variation of resonant frequency is linked to  
231 permittivity through this calibration step [27].

232 Notably, the relative permittivity measurements based on the capacitive  
233 method have several potential sources of uncertainty. These sources are briefly  
234 discussed below.

235 (a) Concrete characteristics: The EM nature of the aggregates, the type  
236 of cement, and the structure's porosity are influential parameters. Also, the  
237 porosity state can affect the relation between permittivity and water content  
238 from one concrete to another.

239 (b) Geometrical/structural characteristics: The curvature of the concrete  
240 structure, surface roughness, and the interface's quality interfere with the qual-  
241 ity of the relative permittivity measurements. Also, the steel reinforcement in

242 the coupling volume of the electrodes is a critical source of measurement un-  
243 certainty due to the different EM characteristics of the reinforcement than the  
244 surrounding concrete. Lastly, the size of the coupling volume, smaller than the  
245 elementary representative volume of a mix like concrete, leads to the potential  
246 uncertainty in the measurements.

247 (c) Environmental characteristics: The permittivity of concrete roughly in-  
248 creases linearly with temperature in the range (5 – 45°C) with a relative slope  
249 of about 0.2 – 0.3%/°C [34]. Also, the permittivity increases linearly with the  
250 volumetric water content with a relative slope of about 0.65 – 0.75%/‰<sub>wc</sub> [27].  
251 Nonetheless, subtracting two successive measurements, one in the air and an-  
252 other in the concrete, removes significant environmental uncertainties.

253 (d) Data acquisition characteristics: The operator influence, the measure-  
254 ment system pressure on concrete and the repeatability of measurements are  
255 potential sources of uncertainty. Also, the regression selection on the calibra-  
256 tion master curve to correlate EM measurements to the relative permittivity  
257 brings potential uncertainty. The trend is linear in the low permittivity range  
258 and exponential for high permittivities [33].

259 In the ANR-SENSO project framework, several NDT experiments are per-  
260 formed on controlled homogeneous concrete slabs [8]. These tests are based on  
261 many different methods such as ultrasonics, radar, capacitive and resistivity.  
262 Their sensitivity and variability are used to evaluate several indicators of con-  
263 crete condition, such as porosity, Young’s modulus, compressive strength at 28  
264 days and water content. Then, an extensive database of about 200,000 data

265 points is provided and studied through statistical data analysis and data fusion.  
266 Relationships between NDT measurements and indicators are determined, and  
267 the variability analysis is presented (refer to [Appendix A](#)).

268 Three vertical lines were tested in the framework of the ENDE project over  
269 the entire height of the structure on the same meshes. The capacitive measure-  
270 ments at vertical lines V1, V2 and V3, are presented in [Figure 5](#). The vertical  
271 lines V1 and V2 are tested at 12 measurement points over the height of about  
272 13 m. The vertical line V3 is tested with 33 measurement points at the height  
273 of about 15 m.

274 The general methodology of investigation while using a GPR consists of  
275 locating the rebars. Once localized, five capacitive measurements are performed  
276 in the neighbourhood of the center of the chosen meshes. The averaged value,  
277 subtracted from the air measurement, is used to estimate the permittivity of  
278 the local area, and the standard deviation of the five measurements is recorded.  
279 The horizontal error bars in the relative permittivity measurement correspond  
280 to the standard deviation of the five measurements points in a chosen mesh.

281 The saturation ratios corresponding to the capacitive measurements are eval-  
282 uated following the surface core regression (see [Figure 3](#)) and are presented in  
283 [Figure 5](#). The horizontal error bars in the saturation ratio estimations corre-  
284 spond to the standard deviation corresponding to the uncertainty coming from  
285 the two following sources. The first corresponds to the local standard deviation  
286 in the relative permittivity at one point. The second one corresponds to the  
287 3.20% (in magnitude) standard deviation obtained from the regression line of

288 the multiple measurements of the center core.

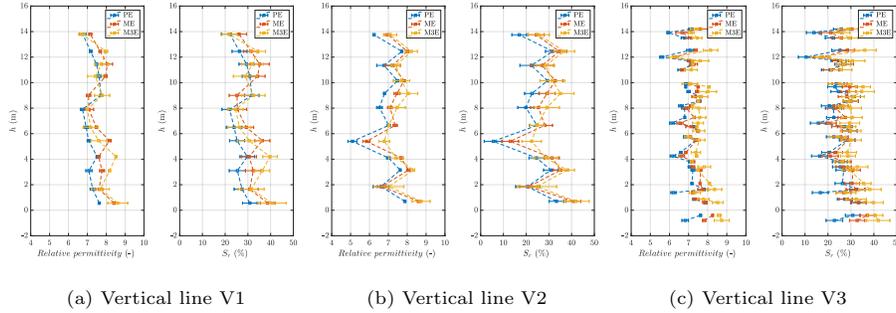


Figure 5: Capacitive measurements and subsequently exploited saturation ratio ( $S_r$ ) profiles on the three vertical lines in the VeRCoRS mock-up outer surface of the inner wall

289 Here, a specific trend on the capacitive measurements is not visible to ex-  
 290 plicitly explore the uncertainties in the measurements with the type of electrode  
 291 used. Nonetheless, a general permittivity gradient with wall depth is observed,  
 292 attributed to natural drying. Similarly, a general trend of saturation ratio de-  
 293 crease vs height is observed. It could be due to the aerial thermal gradient  
 294 remaining inside the structure, accelerating the drying of the concrete structure  
 295 with increasing height. The oscillating experimental measurements over the wall  
 296 height are attributed to the ambient temperature on the concrete pouring day  
 297 and the concreting schedule (mainly three batches per lift and time between  
 298 lifts). These variations affect the 28-days compressive strength and Young's  
 299 modulus, subsequently leading to varying relative permittivity.

300 Overall, the experimental database and the estimation of the saturation ratios  
 301 based on the capacities measurements enable a good understanding of the  
 302 instantaneous drying behaviour of the VeRCoRS mock-up. The detailed explo-

303 ration of the hydric response over the structure’s lifetime calls for a numeri-  
304 cal finite element model of the VeRCoRs mock-up, presented in the following  
305 section. The uncertainty in the model constituent parameters is addressed to  
306 estimate the numerical saturation ratio corresponding to the pressurisation test  
307 VD3 for its comparison with the in-situ measurements.

#### 308 **4. Numerical saturation ratio estimations**

309 This section presents the numerical model framework of the drying phe-  
310 nomenon in the VeRCoRs mock-up. A weakly coupled thermo-hydric modelling  
311 strategy is used. The reference inner NCB temperature and external ambient  
312 temperatures for the thermal exchange are 35°C and 20°C respectively. The  
313 comparatively higher temperature inside results in a lower relative humidity in  
314 the concrete, losing the symmetry through the wall thickness and thus acceler-  
315 ates the drying of concrete. The composition of thermal and hydric phases is  
316 presented hereafter.

##### 317 *4.1. TH constitutive model*

###### 318 *Thermal phase (T)*

319 The temperature field is calculated using the classic heat equation, with no  
320 source term and assuming constant thermal diffusivity.

$$\rho_c C_c^p \frac{\partial T}{\partial t} - \nabla \cdot (\lambda_{hc} \nabla T) = 0 \quad (1)$$

321 Here,  $\rho_c$  is the mass density ( $2368 \text{ kg/m}^3$ ),  $C_c^p$  is the thermal capacity (880  
 322  $\text{J/kg/}^\circ\text{K}$ ) and  $\lambda_{hc}$  is long term thermal conductivity ( $2.5 \text{ J/s/m/}^\circ\text{K}$ ) of con-  
 323 crete.

Limiting conditions of the linear Neumann type are retained via the defini-  
 tion of convective fluxes following Newton's law for the internal and external  
 surfaces of the model, presented in Equation 2.

$$-\vec{q} \cdot \vec{n} = h_{eq,th}(T - T_{ext}) \quad (2)$$

324 Here,  $h_{eq,th}$  is the thermal exchange coefficient ( $10 \text{ J/m}^2/\text{s/}^\circ\text{K}$ ) of concrete.

325 *Hydric phase (H)*

326 In this phase, the evolution of free water content,  $C_{fw}$ , (%) in the concrete's  
 327 volume when exposed to a hydric flow, is presented. Water movement within the  
 328 concrete's connected capillary pores is governed by complex, micro-structural,  
 329 simultaneous and multiphasic processes such as diffusion, evaporation and con-  
 330 densation [35], [36]. The drying kinetics in the concrete is highly dependent on  
 331 the relative humidity ( $RH$ ) within its porosity. Thereby, for a high  $RH$  ( $> 50\%$ ),  
 332 the liquid water diffusivity due to water concentration and saturation rate gra-  
 333 dients in the concrete volume mainly control the drying kinetics. In contrast,  
 334 for a low  $RH$  ( $< 20\%$ ), the vapour diffusivity controls the drying kinetics [37].  
 335 In the framework of the present work, the drying problem is reduced to the  
 336 mass conservation of liquid water only.

$$\frac{\partial C_{fw}}{\partial t} = \nabla \cdot (D(C_{fw}, T) \nabla C_{fw}) \quad (3)$$

Here, the diffusion coefficient ‘ $D$ ’ ( $m^2/s$ ) is computed using a phenomenological approach: a coupled expression from Mensi [11] and Granger [14] models. It is thermo-activated according to the Arrhenius law [12]:

$$D(C_{fw}, T) = A e^{BC_{fw}} \frac{T}{T_{ref}^w} e^{\left[ -\frac{E_a^w}{R} \left( \frac{1}{T} - \frac{1}{T_{ref}^w} \right) \right]} \quad (4)$$

337 Here,  $A$  ( $3.18 \mu m^2/s$ ) and  $B$  (0.057) are the parameters obtained from the  
 338 fitting with the experimental results on concrete mass loss with time for heating  
 339 at  $20^\circ C$  temperature and 50% RH,  $E_a^w$  is the activation energy ( $39000 J/mol$ )  
 340 for drying,  $T_{ref}^w$  ( $15^\circ C$ ) is the reference temperature for thermo-activation of  
 341 the water diffusion and ‘ $R$ ’ is the ideal gas constant.

342 The hydric flow in the boundaries is due to relative humidity ( $RH$ ) between  
 343 the concrete’s exposed edges and the external environment. The presented dry-  
 344 ing model uses the water content as the unknown parameter, while the boundary  
 345 behaviour is expressed by RH. Thus, the two parameters are related through  
 346 the sorption-desorption curve. However, the evolution is different because of  
 347 the different kinetics inducing water loss and gain, meaning that the diffusivity  
 348 factor is not the same during drying and wetting.

349 In this work, it is assumed that only the kinetics of drying is affected for  
 350 the thermal loads considered during the operational phase. It remains valid  
 351 during the period over which the concrete’s RH is higher than the ambient air.  
 352 Also, the VeRCoRs mock-up is a doubled wall structure and therefore, the outer  
 353 face of the TH model of inner-wall is protected from the rain. Therefore, the  
 354 mock-up inner wall boundaries are temperate with no season at a very high

355 RH in the ambient air. Hence, only the desorption curve is taken as sufficient  
 356 representative of the continuous drying. The water content is related to RH via  
 357 the desorption model [9, 38, 39]:

$$C_{fw} = C_{fw,0} \left( 1 + \left( a \ln \left( \frac{1}{RH} \right) \right)^{\frac{1}{1-b}} \right)^{-b} \quad (5)$$

358 Here,  $C_{fw,0}$  is the water content at  $RH = 100\%$  considered representative of  
 359 the one at the end of the hydration process under endogenous conditions. The  
 360 parameters  $a = 7.60$  and  $b = 0.33$  are the empirical coefficients to represent the  
 361 numerical desorption isotherm following the experimental measurement of the  
 362 desorption and the concrete mass loss evolution with time at temperature of  
 363  $20^\circ\text{C}$  and RH of 50% [26]. Notably, during the pressurization tests, the temper-  
 364 ature on the internal face of the inner wall rises to about  $35^\circ\text{C}$ . In contrast, the  
 365 outer face temperatures remain at the NTP conditions varying with different  
 366 seasons. Therefore, a compromise is made to simplify the desorption curve for  
 367 the available limited experimental data at  $20^\circ\text{C}$  reference temperature, repre-  
 368 senting the drying behaviour.

369 Subsequently, the saturation ratio,  $S_r$  (in %), evolving in space,  $\mathbf{x}$  and time,  
 370  $t$  is expressed as the portion of the capillary voids occupied by water, presented  
 371 in Equation 6.

$$S_r(\mathbf{x}, t) = \frac{1}{\phi_V} C_{fw}(\mathbf{x}, t) \quad (6)$$

372 Here,  $\phi_V = 14.6\%$  [1] is the connected capillary voids volume at the end of  
 373 hydration.

374 Following the work of [9], a linear flux of  $RH$  is adopted to define the bound-  
 375 ary conditions at the internal and external surfaces of the model, presented in  
 376 Equation 7. It turns into a nonlinear Neumann type boundary condition as the  
 377  $RH$  is a nonlinear function of the water content.

$$-\vec{q} \cdot \vec{n} = h_{eq,w}(RH - RH_{ext}) \quad (7)$$

378 Here,  $h_{eq,w}$  is the hydric exchange coefficient ( $4.13 \text{ nm/s}$ ) which depends on  
 379 the surface state, the ambient temperature and the vapour pressure, and  $RH_{ext}$   
 380 is the relative humidity of the external environment.

#### 381 4.2. TH structural model

382 The model constitution is implemented on a 2D axisymmetric vertical section  
 383 of the VeRCoRs mock-up in the finite element framework of *Code\_Aster* solver  
 384 [40]. The finite element (FE) mesh is made of linear quadrangular elements  
 385 QUAD4, presented in Figure 6. Triangular linear elements TRIA3 are used to  
 386 provide junctions in geometrically singular areas such as the dome-wall junction.  
 387 The typical size of the FEs is 4 cm, and the mesh comprises 7629 nodes.

388 The in-situ measurements of the ambient air temperature of the internal  
 389 enclosure and the space between enclosures are available only at three locations,  
 390 one located at the level of the gusset ( $z_1 = 4.0 \text{ m}$ ), and the other two at different  
 391 altitudes of the wall ( $z_2 = 11.8 \text{ m}$  and  $z_3 = 19.5 \text{ m}$ ) [1]. Therefore, for the  
 392 temperature fields on internal/external surfaces, a piece-wise linear distribution  
 393 is constructed by dividing the height of the enclosure (noted  $\Omega$ ) into two zones,

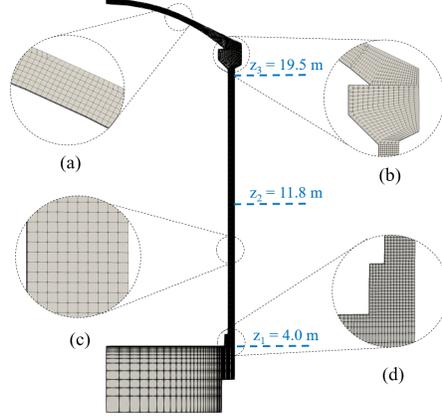


Figure 6: Mesh design of the VeRCoRs mock-up axisymmetric model representing different zones: (a) Dome, (b) dome-wall junction, (c) wall, and (d) gusset

394 presented in Equation 8.

$$\Omega_{ij} = \Omega \cap \{(x, y, z) \in \Omega \mid z_i \leq z \leq z_j\}, \forall i, j \in \{1, 2, 3\}, i < j \quad (8)$$

395 Noting  $T_i^{int}, T_i^{ext}$  as the air temperature measured at altitude  $z_i$  of internal  
 396 and external surfaces respectively, the corresponding air temperature field  $T_{air}^{int}$   
 397 (resp.  $T_{air}^{ext}$ ) is then constructed:

$$T_{air}^{\star}(z, t) = \left( \frac{z_j - z}{z_j - z_i} \right) T_i(t) + \left( \frac{z - z_i}{z_j - z_i} \right) T_j(t) \text{ for } z \in [z_i, z_j], \forall i, j \in \{1, 2, 3\}, i < j \quad (9)$$

398 where  $\star \in \{int, ext\}$ .

399 The subsequent time evolution of the air temperatures in the inner and  
 400 outer surfaces are presented in Figure 7. The temperature variations before the  
 401 heating (at around 1.6 years) are observed similarly in the inner/outer faces.

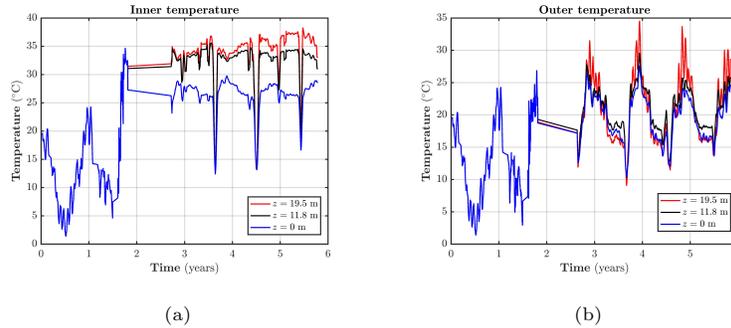


Figure 7: Time evolution of the ambient air temperature measured in the the lifetime of the VeRCoRs mock-up

402 Afterwards, the temperature of inner air is raised and kept approximately at  
 403 35°C. However, warmer air is observed in the top region due to the internal air  
 404 temperature stratification. Subsequently, a higher ambient temperature near  
 405 the dome and a lower near the gusset are recorded. The heating is stopped dur-  
 406 ing simulated unit outages momentarily before the internal pressure is applied in  
 407 the framework of pressurisation tests. The temperature is kept approximately  
 408 at 15°C as seen from the peaks on the inner air temperature profiles. The  
 409 external temperature profiles are seasonal variations controlled and delayed by  
 410 conduction ensured by the outer wall and its inertia. Also, fewer variations over  
 411 the wall height in comparison to the inner wall are observed. Notably, the field  
 412 data is missing between 1.9 to 2.7 years.

413 The temperature field at the times instances of the pressurisation tests is  
 414 presented in Figure 8. In addition, the inner and outer surfaces temperature  
 415 difference and its evolution during the pressurisation test instances are pre-  
 416 sented.

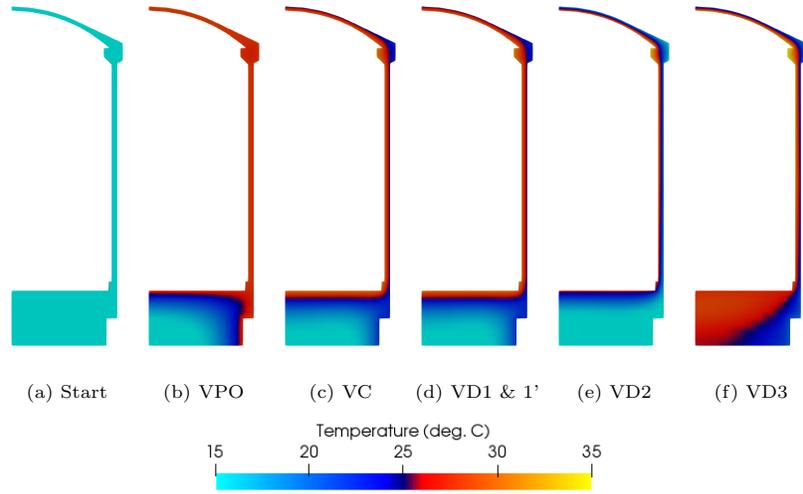


Figure 8: Time evolution of the temperature field in the VeRCoRs mock-up axisymmetric model at different pressurization/depressurisation test instances

417 The temperature field at the pressurization test instance VD3 is further  
 418 explored for its intricacy in different regions of the structure as presented in  
 419 Figure 9. The temperature in the internal and external wall faces in the wall  
 420 region is about 32 °C and 23 °C respectively. The effect of wall thickness  
 421 variation from 40 cm to 60 cm at the gusset level for the temperature evolution  
 422 is observed. Besides the 40cm wall region is the area of interest in this work, the  
 423 TH model is simulated for the mesh without the dome region of the structure  
 424 aimed at computational time reduction. We observe the same temperature  
 425 profile in the wall and gusset regions. Besides the faster computation, removing  
 426 the dome region also simplifies the mesh design comprising only quadrangular  
 427 elements QUAD4. Furthermore, it removes the potential issue of the singularity

428 at the junction for different mesh sizes design.

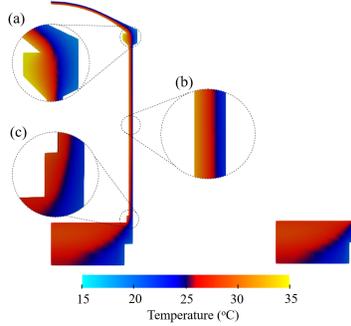


Figure 9: Temperature field at time instance of test VD3 for the full 2D mesh (left) and the mesh without dome region (right), also presenting the details of (a) dome, (b) wall and (c) gusset regions

429 Further, for the model hydric phase input, the in-situ measurements of the  
 430 relative humidity ( $RH_{air}$ ) of the air in the enclosure are not available. Therefore,  
 431 the correlation between the  $RH_{air}$  and the temperature of the ambient air ( $T_{air}$ )  
 432 is expressed by the use of Magnus law (referenced in Bouhjiti et al. [9]), is  
 433 presented in Equation 10.

$$RH_{air} = 163.61 \frac{r}{r + 0.62} e^{-\frac{17.5043 T_{air}}{241.2 + T_{air}}} \quad (10)$$

434 Here, ' $r = 7\text{g/kg}$ ' is the air-water mixing ratio.

435 The *Code\_Aster* FE code allows to create a user-defined non-linear flux only  
 436 in space or in time but not both. Therefore, given this hypothesis, a spatial TH  
 437 boundaries variation is considered to predict the drying behaviour while using  
 438 a time average of the temperature (and thus RH) two successive drying time  
 439 instances.

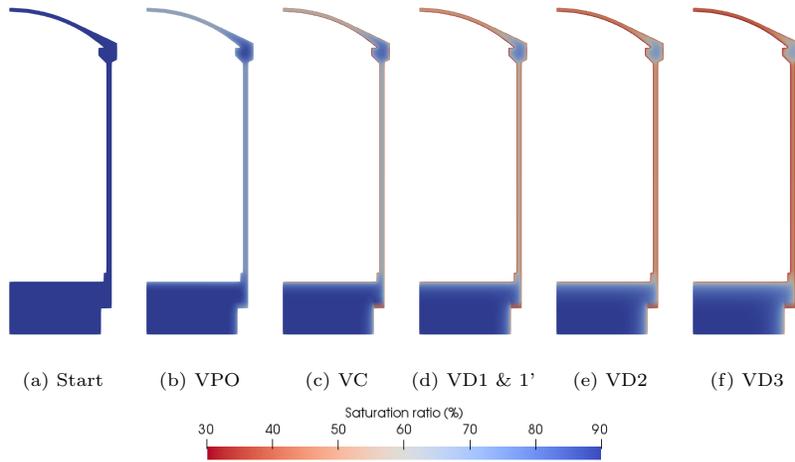


Figure 10: Time evolution of the saturation ratio field in the VeRCoRs mock-up axisymmetric model at different pressurization/depressurisation test instances

440 The time evolution of the degree of water saturation field is given in Fig-  
 441 ure 10. As applicable, an adaptive time scheme linked to the characteristic  
 442 time of the diffusion equation solution is implemented between successive time  
 443 instances. Subsequently, a total of 153 calculation instances for the drying of  
 444 the model over 5.5 years are recorded. The start of drying is considered at 6<sup>th</sup>  
 445 month after the concrete pouring, as representative of the completion of the  
 446 concrete hydration process and early age behaviour. Notably, the  $S_r = 90\%$  is  
 447 thus computed at the start of the drying process, based on Equation 6.

448 Similar to the thermal phase output, the saturation ratio ( $S_r$ ) fields are  
 449 presented in Figure 10 at the time instances of the pressurisation tests. Again,  
 450 a significant drop is observed in the first two years and relatively consistent for  
 451 the later stages when the inner temperature was raised to about 35°C.

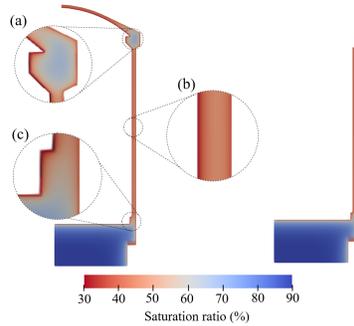


Figure 11: Saturation ratio field at time instance of test VD3 for the full 2D mesh (left) and the mesh without dome region (right), also presenting the details of (a) dome, (b) wall and (c) gusset regions

452 The detail of the saturation field at different zones of VeRCoRs mock-up at  
 453  $t = 4.7$  years are presented in Figure 11. After 4.7 years of drying, the degree  
 454 of saturation at the heart of the current zone is on average equal to 50%. The  
 455 faster drying kinetics of the dome induces a degree of saturation of 45% at the  
 456 core. Because of its thickness, the wall remains more saturated, with a core  
 457 saturation of about 75%. The degree of saturation at the heart of the gusset is  
 458 about 60%. Nearby the gusset step, a saturation of the order of 50% is observed  
 459 due to a thermal bridge effect. Also, the computed saturation ratio field is  
 460 observed the same for computations on a full 2D mesh and without dome mesh.  
 461 Thereby, all computations and analyses presented here onward are performed  
 462 on 2D mesh without dome region.

463 Finally, the mesh design along the wall height is optimised for coherent  $S_r$ ,  
 464 estimations with the least computational time of T and H phases simulations.  
 465 The time optimised mesh element distribution along with the wall thickness is

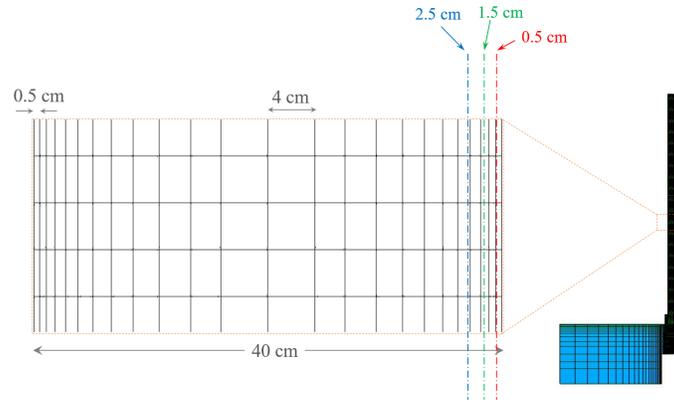


Figure 12: Optimised mesh configuration along wall and three depth levels selected for the degree of saturation computations and comparison with the experimental measurements at the zones of respective depth levels

466 presented in Figure 12. The elements are distributed with varying thicknesses  
 467 from 0.5 cm at the wall edges to 4 cm in the wall center.

468 The time evolution of the saturation ratio from the TH model is explored at  
 469 three vertical lines at depth levels of 0.5cm, 1.5cm and 2.5cm, representing the  
 470 corresponding depths of in-situ electrodes PE, ME and M3E, respectively. Fur-  
 471 thermore, the saturation ratio calculated from the TH model at the test VD3 is  
 472 compared with the saturation ratio estimated from the capacitive measurements.  
 473 Notably, the estimations from the experimental and numerical campaigns are  
 474 independent of each other. Therefore, the blind comparison aims to understand  
 475 the difference in the saturation ratio estimation from the two campaigns and  
 476 discuss the potential sources of the difference and their associated impact with  
 477 the engineering application point of view.

## 478 **5. Blind comparison of experimental and numerical estimations**

479 The drying phenomenon in the wall region is investigated under deterministic  
480 and probabilistic frameworks. It is aimed to estimate the numerical saturation  
481 ratio profile and compare it with the experimental counterpart.

### 482 *5.1. Deterministic numerical vs mean experimental comparison*

483 The TH model is solved deterministically, with the magnitudes of the param-  
484 eters reported in the TH model constitution (see section 4.1). The experimental  
485 measurements of the saturation ratio are the outcome of the capacitive mea-  
486 surements carried out with three types of electrodes, at variable measurement  
487 thicknesses, from 5 mm to 3 cm. The comparison of the calculated saturation  
488 ratios from the TH model at the time instance of the pressurisation test VD3  
489 with the linear regression plot of the mean magnitude of the saturation ratio  
490 from all the capacitive measurements along with wall height for the respective  
491 vertical lines is presented in Figure 13.

492 The calculated degree of saturation does not vary significantly with altitude  
493 as spatially varying material properties and thus spatially varying diffusivity  
494 are not considered in the TH model. On average, the degree of saturation com-  
495 puted from the TH model on the external face is slightly lower ( $\approx 1\%$  at 0.5cm  
496 depth to  $\approx 1.5\%$  at 2.5cm depth) in the top region of the wall than at the  
497 level of the gusset. A similar qualitative mean trend is observed in the experi-  
498 mental measurements. The mean trend given by the capacitive measurements  
499 is determined via a linear regression by ordinary least squares with weighting

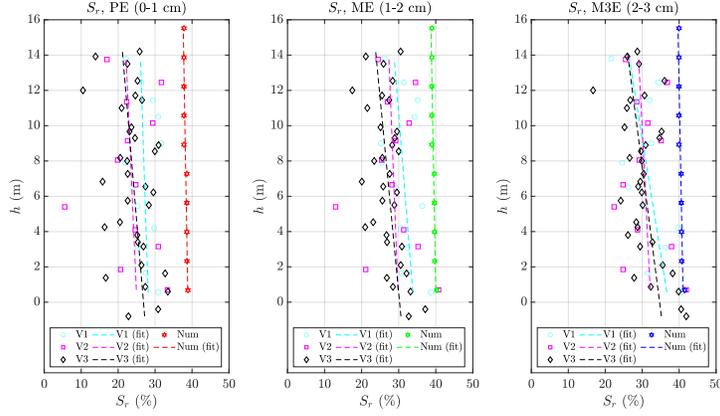


Figure 13: Saturation ratio profile at three depth levels from the deterministic solution of the TH model at the instance of the VD3 pressurisation test and comparison with the mean of the experimental measurements

500 by the inverse of the measurement uncertainties. In general, the slope of the  
 501 mean experimental trend is observed higher than the numerical mean trend.  
 502 Amongst the three vertical lines, line V2 presents the slightest varying slope  
 503 of mean saturation ratio ( $\approx 0.15\%/m$ ) along with the wall height for all three  
 504 depth levels. For vertical line V1, the slope of mean  $S_r$  increases with increasing  
 505 depth level starting from  $\approx 0.20\%/m$  at  $<5mm$  depth, increasing to  $0.35\%/m$  at  
 506 1-2cm depth and lastly further increasing to  $0.70\%/m$  at 2-3cm depth level. For  
 507 vertical line V3, the number of measurements points are higher than the other  
 508 two. However, the slope is intermediate between V1 and V2 measurements and  
 509 is nearly consistent ( $\approx 0.50\%/m$ ). The coherence of experimental measurements  
 510 along three vertical lines is highest with M3E type electrode measurements at  
 511 the same depth level. In contrast, the mean trends from PE and ME electrodes  
 512 are comparatively scattered.

513 Overall, the numerically estimated saturation ratios are 5-10% in magnitude  
514 higher than the mean experimental counterpart. Comparatively, the experimen-  
515 tal measurements approach closer to the numerical estimations with increasing  
516 depth level. The comparative saturation ratio increase with depth level is ob-  
517 served higher for the capacitive measurements than in the numerical model. It is  
518 arguably due to a higher magnitude of the hydric exchange coefficient ( $h_{eq,w}$ ) in  
519 the model (than in reality), resulting in the faster inward movement of the dry-  
520 ing front and hence keeping the rate of saturation ratio increase with depth low.  
521 However, the higher RH at the boundaries provides compensation for the faster  
522 rate of dry front movement. The incumbent reasons for the difference are the  
523 uncertainties in the experimental measurements and approximations in the nu-  
524 merical estimations. From an application point of view, this difference presents  
525 essential information on the critical parameters necessary to identify their ex-  
526 perimental measurements. It also necessarily points out the consequences of the  
527 numerical computations approximation.

528 For example, the RH is averaged between two successive time instances in  
529 numerical computations, assuming the drying kinetics are insignificantly influ-  
530 enced by the varying temperature over time. However, the experimental mea-  
531 surements are carried out at a controlled room temperature ( $\approx 20-25$  °C) at a  
532 specific time instance. So, a potential difference between the ambient air tem-  
533 perature between experimental and numerical estimations subsequently leads to  
534 the different RH and thus different  $S_r$ . However, in this work, the calibration  
535 curve is relevant, assuming that the difference between the lab-scale specimen

536 and in-situ capacitive measurements is not significant.

537       The higher mean magnitude in the numerical estimations can be attributed  
538 to the initial water content taken, assuming an initial saturation ratio of 90%  
539 at the end of the early age of the concrete. If there is a lower bound uncertainly  
540 of 10% in the initial saturation ratio (i.e. if the initial water content occupies  
541 80% porosity), then subsequent saturation ratio magnitude at the timeline of  
542 test VD3 drops by 3.9% on an average.

543       Nonetheless, comparing the numerical model response obtained by a single  
544 set of parameters provides limited and less reliable information. The uncertainty  
545 in the input parameters and the resulting consequence on saturation ratio is  
546 crucial to take into account for the correct and reliable predictions from the TH  
547 model. For this, a stochastic numerical study on the TH model is presented  
548 hereafter.

## 549 *5.2. Stochastic numerical vs experimental comparison*

550       This section presents a stochastic study on the TH model to address the  
551 uncertainty in the input parameters (in terms of the range of their magnitudes)  
552 and their subsequent influence in estimating the saturation ratio profile. First,  
553 a preliminary sensitivity analysis is presented to establish a set of the most  
554 influential parameters on the model response with the least possible computation  
555 cost. Subsequently, an extensive probabilistic sensitivity analysis is presented  
556 using the polynomial chaos expansion (PCE) based surrogate model for the  
557 cost-effective large computations of the TH model. Lastly, the stochastic model  
558 output is compared with the experimental counterpart alongside a discussion

559 on the blind comparison.

Table 2: List of parameters used for the deterministic computation at mean values and characteristic of the uniform distribution retained for the stochastic analysis

Input parameters	Mean magnitude	Uniform distribution bounds		Reference
		Minimum	Maximum	
<i>Thermal (T)</i>				
$\lambda_{hc}$ (kJ/h/m/°C)	4.18	2.51	5.85	[26]
$h_{eq,th}$ (kJ/h/m/°C)	36.0	21.6	50.4	[41]
<i>Hydric (H)</i>				
$S_{r,0}$ (%)	90	80	100	[1]
$\phi_V$ (l/m <sup>3</sup> )	146.0	138.7	153.3	[1]
$A \times 10^{-12}$ (m <sup>2</sup> /s)	3.18	2.54	3.82	
$B \times 10^{-2}$	5.7	4.6	6.8	
$h_{eq,w}$ (nm/s)	4.13	2.68	5.58	
$E_a^w$ (kJ/mol)	39.00	29.25	48.75	[26]

560 A set of 8 input parameters from thermal (T) and hydric (H) phases is  
561 established, presented in Table 2, to explore the influence of each one on satu-  
562 ration ratio computations. Two parameters ( $\lambda_{hc}$  and  $h_{eq,th}$ ) are selected from  
563 the thermal phase where the first one takes into account the uncertainty in  
564 the thermal diffusivity while the second one associates the uncertainty in the  
565 thermal boundary condition. Notably, the thermal capacity parameter ( $C_c^p$ ) is

566 influential for the thermal phase behaviour only at an early age. Hence, it is  
567 not taken into account for the sensitivity study of the long-term behaviour [26].

568 Similarly, six parameters from the hydric phase constitution are selected for  
569 the sensitivity analysis. The initial saturation ratio ( $S_{r,0}$ ) parameter is taken as  
570 an indirect representative of the initial water content ( $C_{fw,0}$ ) to keep  $S_{r,0} \leq 1$   
571 in all the possible input set of the parameters. The uncertainty in the  $C_{fw,0}$   
572 measurement is based on the observed difference between thermogravimetric  
573 analysis estimation [1] and the one based on Powers and Brownyard model [42].  
574 The porosity measurements and the associated uncertainty are selected based  
575 on the reported results in [1]. The mean magnitudes of the parameters  $E_a^w$  and  
576  $h_{eq,w}$  are taken from previous studies [11, 14, 13, 12]. The parameters  $A$  and  
577  $B$  are selected through iterative adjustments of the selected couple of values  
578 ( $A, B$ ), for which the sum of squared residuals is the least in the experimental  
579 mass loss curve [26]. Further, The mean magnitudes of the parameters  $A, B$   
580 and  $h_{eq,w}$  are updated based on the statistical treatment of the hydric phase  
581 by Bayesian calibration strategy. Lastly, the relative humidity of the ambient  
582 air,  $RH_{air}$ , (Equation 10) is estimated based on the temperature measurements  
583 from Equation 9 interpolated over the wall height. Relative humidity estima-  
584 tions are observed insensitive to the uncertainty of  $\pm 15\%$  in the magnitude of  
585 the parameter ‘r’, estimated in the field [1]. Therefore, the parameter ‘r’ and  
586 subsequently, the  $RH_{air}$  is not considered for the sensitivity analysis.

587 Here, for the sensitivity analysis, the ANOVA (ANalysis Of VAriance) frame-  
588 work is adopted, where a parameter is said to be influent (in first-order) if its

589 variations sensibly contribute to the response variance. Sobol' indices [43] sensi-  
590 tivity method belongs to this category. However, it requires many computations  
591 (of order  $10^6$  or more) for correct estimations. Therefore, a priori, one factor  
592 at a time (OFAT) type sensitivity analysis methods are explored to establish  
593 a preliminary understanding of the phenomena with a reasonable computa-  
594 tional cost. The sensitivity analysis module of UQLab [44] presents two OFAT  
595 methods, namely perturbation method and Cotter's method [45], termed as lin-  
596 earisation based methods. Furthermore, the Morris method [46] is used for the  
597 preliminary understanding of the sensitivity of the input variables. The Morris  
598 method is closely similar to Cotter's method but provides a better exhaustive  
599 cover to the entire input space.

600 In this work, first, 1D TH model computations are performed for the sensi-  
601 tivity analysis based on perturbation Cotter and Morris methods. The number  
602 of model evaluations for Morris methods is chosen to be 600, owing to the low  
603 computation time for 1D calculations. Furthermore, the similarity in input  
604 parameters ranking for sensitivity is observed between all three methods. How-  
605 ever, the perturbation method provided minor clear information, and the Morris  
606 method requires many model computations (of order  $> 10^4$ ) for accurate com-  
607 putations. Subsequently, Cotter's method is chosen for preliminary sensitivity  
608 analysis with 'N = 8' input parameters and presented in detail hereafter.

609 The Cotter's method sensitivity analysis for the parameters listed in Table 2  
610 is carried out on the optimised model 2D mesh for ' $S_r$ ' computations. Cotter's  
611 method is a low-cost and straightforward method for ranking input parameters

612 as the Cotter indices. It is based on the assumption that the model is linear or  
 613 linearised around a central value. However, the presented TH model exhibits  
 614 a non-linear behaviour. Therefore, the linearisation assumption oversimplifies  
 615 the model response yet is relevant for the preliminary understanding of the  
 616 sensitivity of the constituent parameters. Besides, it can be applied regardless  
 617 of dependence between the input variables [44]. A brief description of Cotter’s  
 618 method formulation is presented in [Appendix B.1](#).

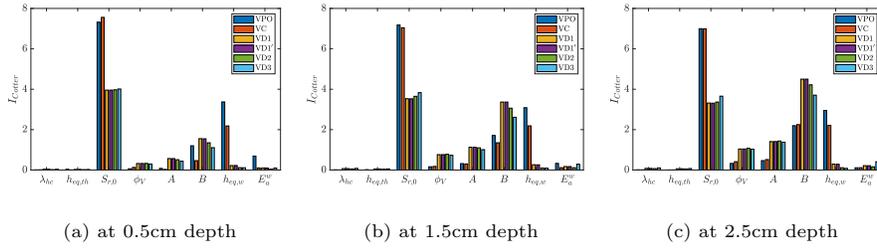


Figure 14: Cotter’s method [45] based Sensitivity analysis of the degree of saturation profile from 2D TH computations on the optimised mesh at mid-wall height for three different depth levels

619 The timeline of the pressurisation tests (indicated in [Figure 2](#)) is used to  
 620 compute the Cotter indices at the equivalent six test instances, presented in  
 621 [Figure 14](#). The indices reflect the negligible effect of variability of the thermal  
 622 phase parameters ( $\lambda_{hc}$  and  $h_{eq,th}$ ) on the saturation ratio profile computation  
 623 for all six test instances. Similarly, in the hydric phase, the variation in the  
 624 activation energy for drying ( $E_a^w$ ) also negligibly affects the saturation ratio  
 625 computation. At 0.5cm depth, the initial saturation ratio ( $S_{r,0}$ ) is observed  
 626 most influential in the first two test instances and constant for the later four

627 test instances. A correlation between the evolution of the saturation ratio field  
628 presented in Figure 10 and the Cotter indices for  $S_{r,0}$  presents direct relevance  
629 where  $S_r$  is higher (in the range 63-67%) for the first two tests and lower (in  
630 the range 38-43%) for the last four tests. A similar trend in Cotter indices is  
631 observed for the available porosity  $\phi_V$ , however, lower in the index magnitude.  
632 Further, the parameters  $A$  and  $B$ , associated with the diffusivity coefficient,  
633 present the opposite trend, being lower for the first two instances and higher  
634 for the latest four instances. The trend presents an indirect correlation between  
635 the significance of the saturation ratio on the diffusion phenomenon.

636 A similar trend is observed at 1.5 and 2.5cm depth levels for the parameter  
637 ranking based on Cotter indices. The pore network parameters ( $s_{r,0}$  and  $\phi_V$ )  
638 present a slight decrease in the sensitivity with increasing depth. It infers the  
639 relatively higher significance of boundary conditions on the hydric exchange.  
640 The parameters  $A$  and  $B$ , related to the diffusion coefficient, present an in-  
641 creasing sensitivity trend with depth and thus indicate faster drying kinetics  
642 near the boundary. The same observation can be accessed from the increasing  
643 sensitivity of the hydric exchange coefficient ( $h_{eq,w}$ ) with depth.

644 Now, having established a preliminary understanding of the sensitivity of the  
645 input parameters, the further stochastic model analysis requires a large number  
646 of computations (e.g. using the MC simulation method). The computational  
647 time is  $\approx 3$  mins for one call to the TH model. Hence, a large number of  
648 model computations are unaffordable yet necessary. Meta-modelling provides  
649 an optimum between the two factors (cost and necessity) for the quality of the

650 computations by substituting the expensive-to-evaluate computational models  
651 with inexpensive-to-evaluate surrogates. In this work, polynomial chaos expan-  
652 sions (PCE) surrogate models are used to approximate the response of the TH  
653 FE model. The PCE is a powerful meta-modelling technique aiming at provid-  
654 ing a functional approximation of a computational model through its spectral  
655 representation on a suitably built basis of orthonormal polynomials [22]. A  
656 brief description related to the PCE surrogate model deployed in this work is  
657 presented in [Appendix B.2](#).

658 The PCE module of UQLab is used to define the sparse PCE surrogate  
659 model configured with the least angle regression (LARS) [47]. The five most  
660 sensitive parameters ( $S_{r,0}$ ,  $\phi_V$ ,  $A$ ,  $B$ ,  $h_{eq,w}$ ) observed from the Cotter indices (see  
661 [Figure 14](#)) at all three depth levels are chosen for the surrogate model creation.

662 The probabilistic distribution of all the parameters is considered to be uni-  
663 form between minimum/maximum bounds, specified in [Table 2](#). The uniform  
664 distribution is chosen because of a weakly informative state of knowledge of the  
665 variability of the input parameters. Classical probability distributions are linked  
666 to well-known families of orthonormal polynomials [48]. The corresponding uni-  
667 variate orthogonal polynomial is of Legendre type for the uniform probability  
668 distribution.

669 The input sample comprising of a set of 100 different values ranging from  
670 the minimum to the maximum magnitude in uniform distribution (see [Table 2](#))  
671 of the five most sensitive parameters are prepared for the PCE creation. UQLab  
672 provides several sampling methods based on MC and quasi MC (such as Sobol',

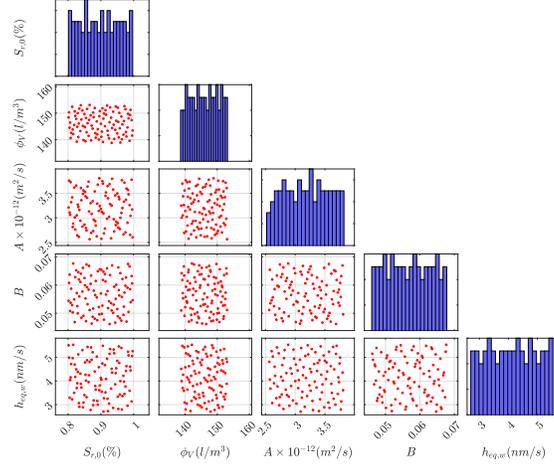


Figure 15: Input sample of size 100 (based on Sobol' sampling method) comprising of five parameters following uniform distribution in their respective ranges of variability for the creation of the polynomial chaos expansion (PCE) based surrogate model

673 Halton) sampling methods [49]. A Sobol' sequence sampling method is used  
 674 to create the input sample, presented in Figure 15, as it provides the best  
 675 parsimoniously filling the input space.

676 The least-angle regression (LARS) method is used to create the PCE meta-  
 677 model truncated to the maximum polynomial degree of  $p = 3$  using a hyperbolic  
 678 truncation scheme with  $q = 1$ . The accuracy of the constructed PCE is esti-  
 679 mated by computing the leave-one-out (LOO) cross-validation error ( $\epsilon_{LOO}$ ).  
 680 This error of order  $10^{-5}$  is reported at all three depth levels for ten validation  
 681 points along with wall height for the time instance of the test VD3. Notably,  
 682 PCE LOO error is of order  $10^{-4}$  for the early pressurization tests (VPO and  
 683 VC) time instances. The observation is in coherence with the stability of the

684 associated physical process of heating and drying. The error magnitude is in the  
 685 acceptable range in the application point of view of the engineering structures  
 686 [50, 51].

687 Additional validation of PCE metamodel accuracy is established by defining  
 688 another independent sample size of 100 for its response comparison from the TH  
 689 and PCE-based surrogate models. The quantitative and qualitative similarity  
 690 of the degree of saturation (i.e.  $Y_{output}$ ) from 100 computations on TH model  
 691 ( $Y_{true}$ ) and its PCE surrogate model ( $Y_{PC}$ ) is presented in Figure 16. The com-  
 692 puted PCE is very accurate with only 100 model calls. It is possibly because the  
 693 study of the process is close to the boundary. Thereby, the boundary condition  
 694 effect in the formulation is directly taken into account by the parameters in the  
 695 boundary. Besides, the 100 model calls provide relative dominance over the de-  
 696 creasing boundary condition effects with increasing depth, keeping the quality  
 697 of the created PCE intact for all three depths.

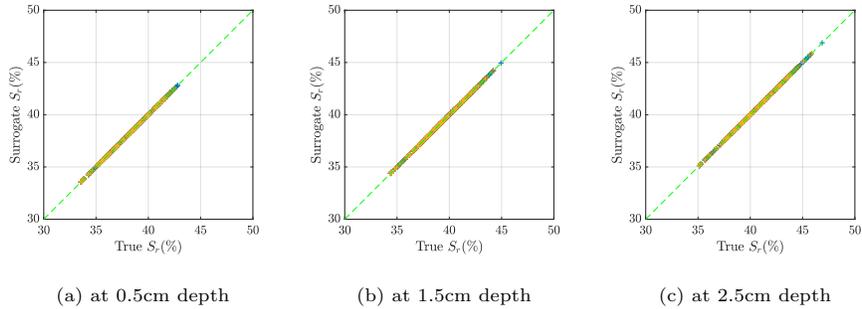


Figure 16: Validation of the polynomial chaos expansion (PCE) based surrogate model using a Monte-Carlo (MC) simulation method based input sample of 100 size

698 The Sobol sensitivity indices are computed from the PCE surrogate model at

699 all three depth levels for the variation of the saturation ratio at the mid-height  
 700 level of the wall at the instance of the pressurization test VD3. The sensitivity  
 701 analysis outcome is presented in Figure 17.

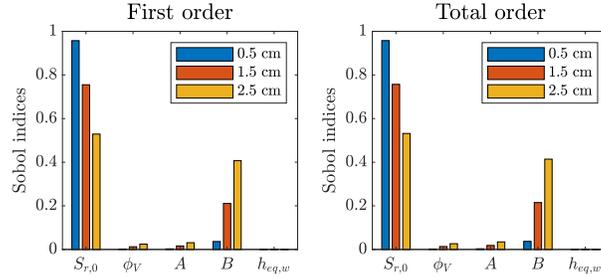


Figure 17: Sobol indices at three depth levels computed from the PCE based surrogate model (at zero cost) of the TH model at the time instance of the pressurization test VD3

702 The qualitative and quantitative estimations from the first order and total  
 703 order Sobol' indices are close. The depth level nearest to the outer surface re-  
 704 flects the highest significance of the initial saturation ratio, progressively reduc-  
 705 ing towards the center of the wall. The response is in line with the observations  
 706 drawn from the preliminary sensitivity analysis based on Cotter's indices (see  
 707 Figure 14). Notably, the dominant effect of the initial conditions (parameter  
 708  $S_{r,0}$ ) in comparison to the boundary conditions (parameter  $h_{eq,w}$ ) on the model  
 709 response may seem counter-intuitive. However, based on the similar trends  
 710 reported from Figure 17 and Figure 14, it is observed that the boundary con-  
 711 ditions are comparatively more influential for the early test instances (VPO  
 712 and VC), while initial conditions still dominate the model response. It can  
 713 be reported that the hydric boundary condition approaches to higher stability  
 714 with the increasing timeline of the VeRCoRs mock-up model. Overall, almost

715 zero Sobol index for the  $h_{eq,w}$  parameter indicates the reliability of the contain-  
716 ment building tightness despite uncertainty and the variability in the external  
717 environmental conditions.

718 The available porosity remains nearly equally influential at all three depth  
719 levels while presenting a trend opposite the initial saturation ratio. The pa-  
720 rameter  $B$ , an indirect representative of the concrete mass loss evolution, is  
721 observed to increase significantly with the increasing depth level (hence increas-  
722 ing the saturation ratio). It infers faster drying kinetics near the external surface  
723 resulting in comparatively quicker stability in the mass loss evolution.

724 The reliability in the TH model response for the saturation ratio evolution,  
725 taking into account the uncertainty in the constitutive parameters, requires  
726 many computations as per the application point of view of the law of large  
727 numbers and the central limit theorem. Therefore, many computations (of  
728 order  $10^6$ ) are carried out using the PCE metamodel to estimate the probability  
729 density function (PDF) of the degree of saturation at three different depths along  
730 with wall height. Three wall height levels *i.e.* bottom = 0 m, mid = 6.6m and  
731 top = 13.2m with an offset of 4.68m from global height coordinates of wall  
732 bottom are chosen to plot the PDF as a representative of the entire wall height  
733 response. The computed PDFs are presented in Figure 18.

734 The overall response at a particular depth level is qualitatively similar at  
735 all three wall height levels. Therefore, indirectly presenting the spatial homo-  
736 geneity consideration of the material parameters in the TH model. At 0.5cm  
737 depth level, the PDF presents a plateau of bandwidth about 6% (between 36%

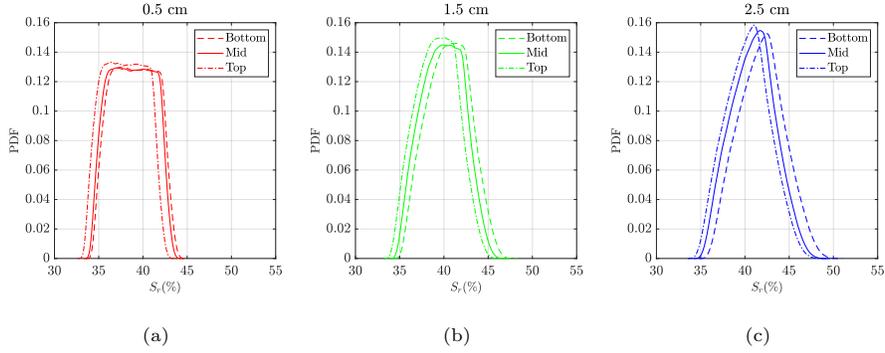


Figure 18: Probability density function (PDF) for the degree of saturation for the test instance of VD3 at different height and depth intervals along the wall obtained from  $10^6$  model computations following a Monte-Carlo (MC) simulation method

738 and 41%) saturation ratio. In comparison, the bandwidth of this plateau de-  
 739 creases with increasing depth level to about 3% at 1.5cm depth and  $< 1.5\%$  at  
 740 2.5cm depth level. The decreasing trend reflects the increasing stability in the  
 741 hydric exchange between the wall and outer environment with increasing depth.  
 742 Also, the boundary condition effect in the TH model constitution presents the  
 743 explanation of the plateau at the 0.5cm depth level. The correlation between  
 744 the initial saturation ratio ( $S_{r,0}$ ) and hydric exchange coefficient ( $h_{eq,w}$ ) states  
 745 that to obtain a similar RH, either a higher or a lower magnitude of both pa-  
 746 rameters is needed. Therefore, the varying magnitude of both parameters in  
 747  $10^6$  computations incorporates the effect of the boundary (via  $h_{eq,w}$ ) to a com-  
 748 paratively greatest extent. The arithmetic mean of 38.71%, 39.92% and 40.98%  
 749 at the mid-height wall level for 0.5cm, 1.5cm and 2.5cm depth respectively are  
 750 reported from  $10^6$  computations based on the MC simulation method.

751 Further, the confidence interval of the saturation ratio magnitude is estab-

752 lished using the cumulative density function (CDF) of  $10^6$  computations, pre-  
 753 sented in Figure 19. Here, for depth level 0.5cm (see Figure 19a), the confidence  
 754 interval at three height and depth levels is computed as 90% probable output  
 755 by making a threshold for the zone of uncertainty (Z.U.) at the lower and upper  
 756 5% probable outcomes. The range of  $S_r$  for wall bottom and top height levels  
 757 is estimated in the similar guidelines and subsequently extended to the 1.5 cm  
 758 (Figure 19b) and 2.5 cm (Figure 19c) depths for the three height levels.

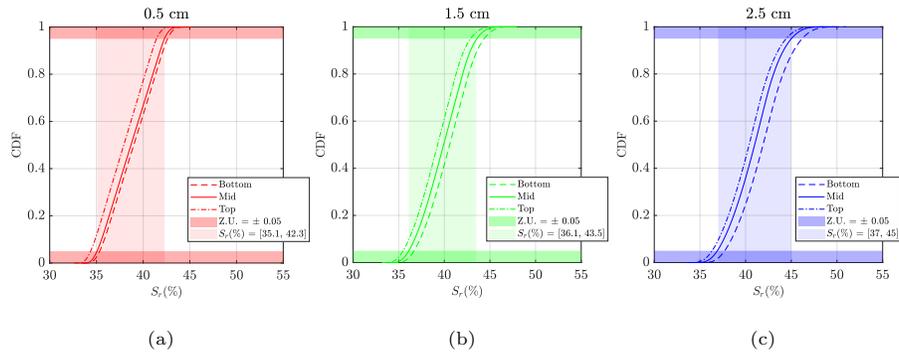


Figure 19: Cumulative density function (CDF) for the degree of saturation for the test instance of VD3 at different height and depth intervals along the wall obtained from  $10^6$  model computations following a Monte-Carlo (MC) simulation method

759 The blind comparison of  $S_r$  along wall height between field measurements at  
 760 three depth ranges with PE, ME and M3E electrodes and numerical stochastic  
 761 computations at three wall depths levels are presented in Figure 20. Here, two  
 762 numerical computational parameters are presented, the arithmetic mean ( $\mu$ ) of  
 763  $10^6$  computations for ten height levels and the standard deviation ( $\sigma$ ) in the  
 764 form of the confidence interval  $S_r$  obtained from the respective CDFs. Also,  
 765 the uncertainty in the capacitive measurements based saturation ratio (*i.e.* un-

766 certainty on the estimate of the mean value) is presented by horizontal error  
767 bars at each measurement point. The numerically estimated saturation ratios  
768 are higher than the experimental counterpart, while the experimental measure-  
769 ments approach the numerical estimations with increasing depth levels. The  
770 experimental measurements at all depth levels range from 0-50% as extreme  
771 limits, while most of the measurements are 20-40% range. The numerically es-  
772 timated  $S_r$  presents a narrower range of about 8% in magnitude at all three  
773 depth levels with nearly similar magnitudes over the wall height with a decreas-  
774 ing gradient of 0.14%/m between wall bottom and top. A brief discussion on  
775 Figure 20 outcomes to establish a link between independent experimental and  
776 numerical campaigns is presented hereafter.

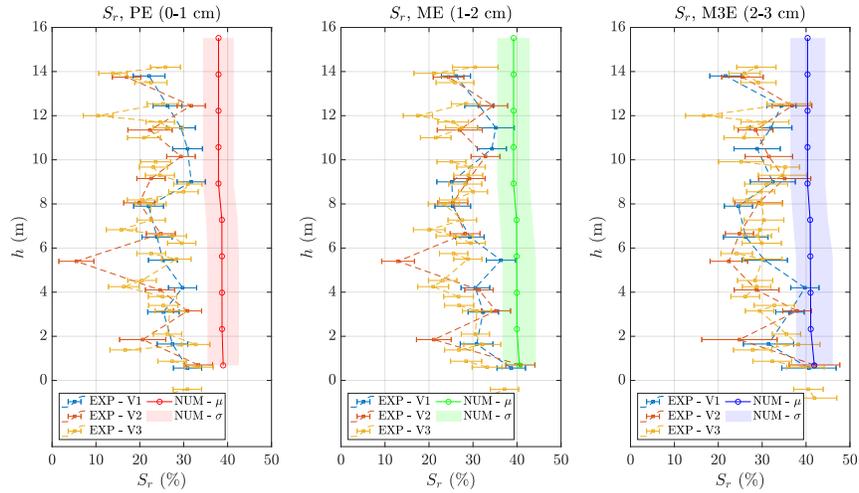


Figure 20: Comparison of experimental data exploited from three electrodes PE, ME and M3E with stochastic numerical computations at depths 0.5cm, 1.5cm and 2.5cm respectively for the saturation ratio estimations corresponding to the VD3 pressurization/depressurisation test instance

777 First, the uncertainty in the magnitude of the experimental porosity mea-  
778 surements has a direct impact on the reported saturation ratios in Figure 3.  
779 The center core porosity is reported 15.8% (average from eight cores), while the  
780 surface porosity is 14.5%. The evolution (decrease) of the porosity towards the  
781 surface suggests that the porosity on the three first centimetres could join about  
782 13.4%. Thus, this hypothesis would increase the experimentally estimated sat-  
783 uration ratio by 2 to 2.5% in magnitude. Besides, the numerical mean porosity  
784 is taken as 14.6%, which is associated with the experimental porosity obtained  
785 from the surface cores. If the numerical mean porosity is changed to 15.8% (cor-  
786 responding to the center core measurements), the overall stochastic TH model  
787 response decreases the  $S_r$  measurements by less than 1% in magnitude. Hence,  
788 the uncertainty in the numerical mean porosity measurements is not significant  
789 for the numerical stochastic computations. Besides, the experimental porosity  
790 measurements are sensitive to the experimental  $S_r$  computation due to their  
791 impact on the calibration curve. Increasing the surface porosity to 15.8% (from  
792 14.5%) shall further reduce the experimental mean saturation ratio magnitude  
793 by 2.5 to 3% on average over different depth levels. Therefore, a porosity in-  
794 crease from 14.5% to 15.8% reduces the experimentally estimated saturation  
795 ratio magnitude by two to three times more than the numerical counterpart.

796 Second, the uncertainty in the magnitude of the constitutive hydric phase  
797 parameters is well identified as presented in the stochastic numerical model.  
798 However, the drying behaviour, more specifically the hydric exchange between  
799 the outer wall surface and the environment, is defined by the desorption model

800 presented in Equation 5. The desorption model parameters ‘a’ and ‘b’ are com-  
801 puted to represent the numerical desorption isotherm following the single point  
802 experimental measurement of the desorption and the concrete mass loss evo-  
803 lution with time at temperature of 20°C and RH of 50% [26]. Comparing the  
804 desorption isotherm database available for different concretes presents the signif-  
805 icance of the constituent parameters ‘a’ and ‘b’. Numerically, an increase of the  
806 two parameters by 10% decreases the numerical mean  $S_r$  to about 6.5% in mag-  
807 nitude at all three depth levels at the time instance of the VD3 test. Thereby,  
808 the updated desorption model shall reduce the difference between experiment  
809 and numerical saturation ratio estimations. Besides, the TH model takes into  
810 account the only reference we know for the desorption behaviour, defined at  
811 the temperature of 20°C. However, the ambient air temperatures vary between  
812 about 10°C to 35°C in the outer surface and likewise vary between about 5°C to  
813 38°C in the inner surface (see Figure 7) over the lifetime of the VeRCoRs mock-  
814 up. In general, a lower reference temperature desorption isotherm shall lead to  
815 further higher estimations of the numerical saturation ratios and vice-versa.

816 Lastly, it is forbidden to extract the concrete cores from the VeRCoRs  
817 mock-up containment structure where the non-destructive measurements are  
818 performed. This restriction imposes a contradiction to the calibration recom-  
819 mendations [31] for the conversion of the non-destructive measurements into the  
820 degree of saturation for the VeRCoRs mock-up. In this work, the calibration  
821 procedure is carried out on concrete cores that are taken from a similar concrete  
822 mix that is poured and cured in the laboratory in different conditions than the

823 real structure. Therefore, the absence of a ‘true’ calibration curve potentially  
824 induces a global under-evaluation of the experimentally evaluated saturation  
825 ratios.

826 Nonetheless, for the blind comparison, the available data on the porosity  
827 measurements, desorption model and the calibration curve is used. Therefore,  
828 the results reported in Figure 20 are kept intact. Overall, the difference in the  
829 estimations from the two independent campaigns highlight the sensitivity of  
830 experimental calibration and numerical approximations on the saturation ratio  
831 estimations.

## 832 **6. Conclusions**

833 Experimental and numerical estimation of the saturation ratios in the VeR-  
834 CoRs NCB structure, and their blind comparison and discussion, are presented.  
835 The in-situ capacitive measurements are carried out along three vertical lines  
836 along the outer surface of the inner wall of VeRCoRs mock-up. This NDT  
837 technique associated with three-electrode probes presented the experimental es-  
838 timate of the saturation ratio on the first centimetres of the wall. A weakly  
839 coupled thermal and hydric model of an asymmetric vertical sector of VeRCoRs  
840 mock-up is presented for the deterministic and stochastic numerical estimations  
841 of the saturation ratio.

842 A set of eight input parameters is prepared for this study over six-time in-  
843 stances representative of the pressurising/depressurisation tests on VeRCoRs  
844 mock-up. Cotter’s method based sensitivity analysis presented a preliminary

845 ranking of the influence of each parameter. The variation in the thermal phase  
846 parameters is concluded least influential in the saturation ratio estimation. The  
847 hydric phase parameters, namely initial water content ( $C_{fw,0}$ ), free water ac-  
848 cessible porosity ( $\phi_V$ ), diffusivity coefficients ( $A$  and  $B$ ) and hydric exchange  
849 coefficient ( $h_{eq,w}$ ) are concluded as most influential parameters for saturation  
850 ratio estimations from the TH model.

851 Further, the mesh design along the wall is optimised based on the consistency  
852 in the saturation ratio estimations. Finally, the knowledge of each parameter's  
853 influence and the optimised mesh design are incubated for the probabilistic  
854 analysis of the degree of saturation estimations from 3D TH model computation.

855 A polynomial chaos expansion (PCE) based surrogate model of the 3D TH  
856 model is created to enable a large number of computations (of order  $> 10^6$ ), with  
857 practically zero cost, for probabilistic analysis of the saturation ratio. Compar-  
858 ing numerical estimations at the respective depth levels with the in-situ mea-  
859 surements at the latest pressurisation test instance presented consistent results.  
860 In an entirely blind approach, the minimum mean difference between the com-  
861 puted saturation ratio in the two approaches remains at about 6% in magnitude.  
862 However, the difference potentially reduces to 5% for the numerical computa-  
863 tions with the mean porosity of 15.8% (instead of 14.6%). The difference further  
864 reduces to about 1% with updated desorption model parameters.

865 Overall, the experimental and numerical estimations are in close agreement  
866 with each other for the behaviour at the outer surface of the containment wall.  
867 Moreover, drying behaviour at the central regions of the wall is also crucial to the

868 durability of the containment structures. While the capacitive measurements are  
869 in the development phase for the in-situ measurements at the wall center regions,  
870 the presented TH model response can be reliably used to access the drying  
871 behaviour at the central regions. An update in the model desorption isotherm  
872 from a brand new experimental database shall increase the reliability of the TH  
873 stochastic model response. Besides, a larger input sample may be required to  
874 correctly create an accurate PCE based surrogate model of the drying behaviour  
875 at the wall center region due to its distance from the boundaries. Eventually,  
876 a complementary study could also consider the quantification and the effect of  
877 the variability of a larger number of input parameters.

## 878 **Acknowledgments**

879 The authors acknowledge the funding support from France's National Re-  
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881 0009 and ProjetIA-11- RSNR-0012) for this work.

## 882 **Appendix A. The variability considered in the in-situ measurements**

883 Different types of variability were considered concerning on-site measure-  
884 ments. The first variability (Var1) is modelled linked to the repeatability of  
885 numerous measurements at the same point. The second variability (Var2) cor-  
886 responds to the measurement variability in the same area assumed as homoge-  
887 neous. The third variability (Var3) is the variability between different homoge-  
888 neous areas of the same concrete batch. The last variability (Var4) considered is

889 the variability of fabrication consisting of comparing the measurements obtained  
 890 on two identical concretes but fabricated in different batches and at different  
 891 times.

892 Variance values presented in Table A.3 correspond to averages from six con-  
 893 crete mixes having the same components (rolled siliceous aggregates, granulom-  
 894 etry, cement CEM I 52.5 NCalcia) but different water/cement ratios from 0.31  
 895 to 0.9, inducing different porosities. During this ANR-SENSO project [8], only  
 896 electrodes PE and ME were tested, M3E being designed several years later.

Table A.3: Variances of permittivity (-) related to capacitive electrodes measured in the project ANR-SENSO

Electrode	Variance	Saturated state	Dry state
ine	Var1	$9.43 \times 10^{-4}$	$8.33 \times 10^{-6}$
	Var2	$4.10 \times 10^{-3}$	$1.68 \times 10^{-5}$
ME	Var3	$2.67 \times 10^{-1}$	$1.08 \times 10^{-1}$
	Var4	3.54	$3.23 \times 10^{-1}$
	Var1	$2.11 \times 10^{-2}$	$1.16 \times 10^{-4}$
PE	Var2	$3.20 \times 10^{-2}$	$8.90 \times 10^{-5}$
	Var3	1.47	$8.91 \times 10^{-2}$
	Var4	2.18	$2.41 \times 10^{-1}$

897 The order of difference between variances related to punctual measurements  
 898 (Var1 and Var2) and those corresponding to regional or global measurements  
 899 (Var3 and Var4) can be seen. This is because these data are obtained in sim-

900 ilar indoor conditions. Thus, the variance is only due to the concrete and the  
 901 electronics of the capacitive sensor variabilities. Furthermore, the variability  
 902 increase for saturated concretes can be interpreted as porosity variations.

## 903 **Appendix B. Theory of the implemented stochastic methods**

### 904 *Appendix B.1. Cotter's sensitivity analysis method*

905 Consider the input vector of the set of eight TH model parameters as  $\mathbf{x} =$   
 906  $\{x_1, \dots, x_8\}^T \in \mathcal{D}_x$ . Each input variable,  $X_i$ , is varied between its minimum,  
 907  $x_i^-$ , and maximum,  $x_i^+$ , magnitudes following a systematic sequence of model  
 908 evaluations with  $N = 8$  input variables as listed hereafter. So, for an equivalent  
 909 mathematical model  $\mathcal{M}(X)$  of the TH FE model, Cotter's method is imple-  
 910 mented as follows:

- 911 • One run with all variables at their minimum values:  $S_r^1 = \mathcal{M}(x_1^-, \dots, x_8^-)$
- 912 • Eight runs at minimum magnitude, switching one variable at a time to its  
 913 maximum magnitude:  $S_r^{i+1} = \mathcal{M}(x_1^-, \dots, x_i^+, \dots, x_8^-), i = 1, \dots, 8$
- 914 • Eight runs at maximum magnitude, switching one variable at a time to  
 915 its minimum magnitude:  $S_r^{i+9} = \mathcal{M}(x_1^+, \dots, x_i^-, \dots, x_8^+), i = 1, \dots, 8$
- 916 • One run with all variables at their maximum values:  $S_r^{18} = \mathcal{M}(x_1^+, \dots, x_8^+)$

917 Here,  $\mathbf{x} = \{x_1, \dots, x_8\}^T = \{\lambda_{hc}, h_{eq,th}, C_{fw,0}, \phi_V, A, B, h_{eq,w}, E_a^w\}^T$  is the  
 918 input variable vector.

919 The computed saturation ratio ( $S_r$ ) from 18 model evaluations is processed  
 920 at each input variable  $X_i$ , where  $i \in [1, 8]$  for the expectation of the importance

921 of the odd and even order effects. Equation B.1 presents the formulation of the  
 922 odd ( $C_o(i)$ ) and even ( $C_e(i)$ ) order effects expectation for each input variable.

$$\begin{aligned} C_o(i) &= \frac{1}{4} \left[ (S_r^{18} - S_r^{i+9}) + (S_r^{i+1} - S_r^1) \right] \\ C_e(i) &= \frac{1}{4} \left[ (S_r^{18} - S_r^{i+9}) - (S_r^{i+1} - S_r^1) \right] \end{aligned} \quad (\text{B.1})$$

923 Subsequently, the importance of each variable is measured by the Cotter  
 924 index ( $I_{Cotter}$ ):

$$I_{Cotter}(i) = |C_o(i)| + |C_e(i)| \quad (\text{B.2})$$

925 *Appendix B.2. PCE surrogate model*

926 Consider TH model represented by a  $\mathcal{M}(\mathbf{X})$  as an equivalent mathemati-  
 927 cal model. Here,  $\mathbf{X} \in \mathbb{R}^M$  is a random vector with independent components  
 928 described by the joint probability density function (PDF)  $f_{\mathbf{X}}$ . Consider also a  
 929 finite variance computational model as a map  $Y = \mathcal{M}(\mathbf{X})$ , with  $Y \in \mathbb{R}$  such  
 930 that:

$$\mathbb{E} \left[ Y^2 \right] = \int_{\mathcal{D}_{\mathbf{X}}} \mathcal{M}(\mathbf{x})^2 f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} < \infty \quad (\text{B.3})$$

931 Then, under the assumption of Equation B.3, the PCE of  $\mathcal{M}(\mathbf{X})$  is defined  
 932 as:

$$Y = \mathcal{M}(\mathbf{X}) = \sum_{\alpha \in \mathbb{N}^M} y_{\alpha} \Psi_{\alpha}(\mathbf{X}) \quad (\text{B.4})$$

933 where, the  $\Psi_{\alpha}(\mathbf{X})$  are multivariate polynomials orthonormal with respect to  
 934  $f_{\mathbf{X}}$ ,  $\alpha \in \mathbb{N}^M$  is a multi-index that identifies the components of the multivariate  
 935 polynomials  $\Psi_{\alpha}$  and the  $y_{\alpha} \in \mathbb{R}$  are the corresponding coefficients. In practical  
 936 applications, the sum in Equation B.4 needs to be truncated to a finite sum by  
 937 introducing the truncated polynomial chaos expansion:

$$\mathcal{M}(\mathbf{X}) \approx \mathcal{M}^{PC}(\mathbf{X}) = \sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(\mathbf{X}) \quad (\text{B.5})$$

938 where,  $\mathcal{A} \subset \mathbb{N}^M$  is the set of selected multi-indices of multivariate polyno-  
 939 mials.

940 In this work, the least-angle regression (LARS) method is used to create the  
 941 PCE metamodel truncated to the maximum polynomial degree of  $p = 3$  using  
 942 hyperbolic truncation scheme with  $q = 1$ .

$$\mathcal{A}^{M,p,q} = \{\alpha \in \mathcal{A}^{M,p} : \|\alpha\|_q \leq p\}, \text{ where } \|\alpha\|_q = \left( \sum_{i=1}^M \alpha_i^q \right)^{1/q} \quad (\text{B.6})$$

943 The accuracy of the constructed PCE is estimated by computing the leave-  
 944 one-out (LOO) cross-validation error ( $\epsilon_{LOO}$ ). It consists in building  $N$  meta-  
 945 models  $\mathcal{M}^{PC \setminus i}$ , each one created on a reduced experimental design  $\mathfrak{X} \setminus \mathbf{x}^{(i)} =$   
 946  $\mathbf{x}^{\{j\}, j = 1, \dots, N, j \neq i\}$  and comparing its prediction on the excluded point  
 947  $\mathbf{x}^{(i)}$  with the real value  $y^{(i)}$ . The leave-one-cross-validation error can be writ-

948 ten as:

$$\epsilon_{LOO} = \frac{\sum_{i=1}^N \left( \mathcal{M}(\mathbf{x}^{(i)}) - \mathcal{M}^{PC \setminus i}(\mathbf{x}^{(i)}) \right)^2}{\sum_{i=1}^N \left( \mathcal{M}(\mathbf{x}^{(i)}) - \hat{\mu}_Y \right)^2} \quad (\text{B.7})$$

949 where,  $\hat{\mu}_Y$  is the mean of the experimental design sample.

## 950 References

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