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## **1** Analysis of water transport in unsaturated conditions:

## 2 comparison between labcrete and fieldcrete

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#### 8 Abstract

- 9 The differences in unsaturated permeability between concrete prepared in the laboratory
- 10 (labcrete) and on a real construction site (fieldcrete) were investigated experimentally and
- 11 using inverse analysis. Although more porous, the fieldcrete specimens were shown to have an
- 12 average permeability very close to the labcrete ones. The fieldcrete permeabilities also exhibited
- 13 more variability than the labcrete ones. Numerical simulations performed on 3D reconstructed
- 14 concrete specimens showed that differences in coarse aggregate distribution cannot explain the
- 15 variability observed at the macroscopic scale and that an important part may originate from the
- 16 properties of mortar matrix.
- 17 Keywords: labcrete; fieldcrete; permeability; inverse analysis; 3D mesostructure.

## 18 1. Introduction

- 19 The amount of evaporable water that is present in the porosity of concrete is of paramount
- 20 importance for the durability of reinforced concrete structures: (1) because it influences the
- 21 concrete transport properties and then the ingress rate of aggressive species such as CO<sub>2</sub> or
- 22 chlorides [1–5]; (2) because the poral solution is the medium that allows chemical reactions to

occur such as carbonation or rebar corrosion [6–8] and also (3) because the loss of water
induces shrinkage and possibly cracking [9–11] Describing water exchange between a concrete
structure and the surrounding environment is then the first and inevitable step towards
durability assessment.

27 Among the data needed to describe water transport, the permeability is of first importance: it 28 accounts for the ability of a fluid (water in our case) to pass through concrete due to pressure 29 gradient. Permeability is considered as a relevant durability index for service-life prediction 30 [12–16] and is measured to verify whether the concrete composition complies with the 31 specifications. To this end, characterization tests are generally performed using specimens 32 prepared in the laboratory ('labcrete'). This approach may be regarded as inconsistent because 33 it does not account for the properties of the concrete that is prepared and used onsite 34 ('fieldcrete') [17,18]. Labcrete specimens are generally prepared with great care by experienced 35 technicians and/or scientists using batches of small volume, in controlled environmental 36 conditions and are carefully vibrated and cured whereas fieldcrete is generally prepared in 37 much larger batches in concrete plants in uncontrolled environmental conditions before further 38 use by onsite workers [18,19]. Fieldcretes are then likely to be of lower quality than labcretes in 39 terms of mechanical as well as durability properties; the question is how much?

40 There are very few studies in the literature that compare the properties of labcrete and 41 fieldcrete. However, fieldcretes are known to exhibit reduced compressive strength compared to 42 labcretes and the difference is about 10-15% [20,21]. Unexpectedly, no significant differences in 43 chloride diffusion coefficient between laboratory and field measurements were obtained over a 44 large panel of concretes by [22,23], indicating that fieldcretes and labcretes would be similar in 45 terms of diffusion properties. The available results about permeability tell a different story. 46 Using gas, the permeability of fieldcrete was shown to be greater than that of the labcrete up to 47 four times [24–26]. The same applies to the studies of Diaz *et al.* [27] who used the Torrent 48 permeameter to measure the permeability of low-carbon concrete elements exposed to marine 49 environment *in situ* as well as companion specimens in the laboratory. The field measurements

50 were up to 8 times higher than the laboratory ones. This discrepancy may be due to differences 51 in properties of lab- and fieldcrete but also to differences in water content between the 52 laboratory and field specimens [28] and to the absence of proper cure for the fieldcrete [29,30]. 53 The objective of this study is to investigate the differences in water permeability in unsaturated 54 conditions between a labcrete (concrete prepared and cured in the laboratory) and the 55 corresponding fieldcrete (same formulation of concrete prepared on a construction site); this is 56 obviously lacking in the scientific literature. The influence of the on-site cure (*e.g.* early-age 57 drying) and structural effects (*e.g.* cracking) is not addressed in this article and should be the 58 subject of a further study. Specifically, mass loss due to drying of several specimens from 59 saturation up to 30% of relative humidity is measured. The results are then used for identifying 60 by inverse analysis and comparing the parameters of a classical model describing the water 61 transfer via a single mass balance equation. Besides this experimental procedure, one-62 dimensional numerical simulations are performed to analyze the sensitivity of the saturation 63 profiles towards the identified materials parameters. Further, 3D simulations on mesoscale 64 concrete specimens exhibiting different aggregate distributions are performed to investigate 65 more precisely local effects due to the presence of aggregates on the saturation degree.

## 66 2. Material and methods

#### 67 2.1. Concrete

The concrete used in this study was designed by the Belgian agency for radioactive waste and enriched fissile materials (ONDRAF-NIRAS<sup>1</sup>) in the framework of a project of Low-Level radioactive waste surface disposal in Dessel, Belgium (Ondraf-Niras, 2010). It is a modern concrete including CEM I (Ordinary Portland Cement) with a water-to-cement ratio of 0.47. The superplasticizer (Masterglenium<sup>®</sup> 27) content was adjusted so that the slump of the fresh mix would reach 19 cm. The average compressive strength at 28 days is equal to 49 MPa using

<sup>&</sup>lt;sup>1</sup> http://www.nirond.be

74 cylinders (68 MPa was obtained using cubes). A large experimental campaign was undertaken at 75 the Eduardo Torroja Institute ( $IeTcc^2$ ) in which many characterization tests were conducted on a 76 preliminary but very similar composition [31] along with a sensitivity analysis at the Belgian 77 Building Research Institute [32], demonstrating its robustness. Among all of them the first 78 desorption isotherm was acquired. This concrete (Table 1) was studied in laboratory and was 79 also produced in industrial conditions for the realization of test panels (11 m height, 3 m long) to 80 verify its feasibility for the construction of surface disposal modules in Dessel. Up to this day, three test panels have been erected with this composition, each of them containing about 25 m<sup>3</sup> 81 82 concrete. About 6 to 10 batches were furnished during the construction of each test panel. The 83 fieldcrete used in this study was produced during one of these test panels. The cubes were 84 fabricated on-site by the site workers. They were unmolded the day after casting and they were 85 then kept in a humid chamber (RH>95%, ca. 20°C) for 28 days. After that, the specimens were 86 kept under water at ambient temperature for multiple months before use. 87 In the laboratory the concrete (labcrete) was mixed in small batches (30 L) and cylindrical 88 specimens (Ø11×H22 cm) were prepared that were normally vibrated and then kept in their

- 89 sealed molds before use.
- 90

#### Table 1 – composition of the concrete

Compound	Nature	Quantity (kg/m <sup>3</sup> )
Low-heat cement	CEM I 42.5 LH	360
Filler	Limestone (Calcitec)	40
Water		169
Gravel 6/20 mm	Limestone	472
Gravel 6/14 mm	Limestone	200
Gravel 2/6 mm	Limestone	417
Sand 0/4 mm	Limestone	721
Superplasticizer	Glenium 27 (BASF)	1.8 (0.5 wt% of cement)

91

<sup>&</sup>lt;sup>2</sup> http://www.ietcc.csic.es/index.php/en/

#### 92 2.2. Methods

93 Four mature labcrete specimens ( $\emptyset$ 11×H22 cm), that were kept two years in their sealed molds 94 after casting, were cored to generate 4 smaller cylinders ( $\emptyset$ 6×H22 cm). Top and bottom ends, 95 whose properties may differ from the bulk [33–36], were sawn and thrown away. This resulted 96 in four new cylinders ( $\emptyset$ 6×H15 cm) that assumedly exhibited uniform properties. In the same 97 way, five mature fieldcrete cubes  $(15 \times 15 \times 15 \text{ cm})$ , originating from five different batches, were 98 cored to generate two smaller cylinders ( $\emptyset$ 6×H15 cm): 2 cylinders per cube. They were cut as 99 described above resulting in ten new cylinders ( $Ø6 \times H11$  cm). 100 All the specimens were resaturated under water and vacuum [37] and the volume and density of each specimen were measured using the buoyancy method (Table 2). All the saturated cylinders 101 102 were introduced in a climatic chamber at 25 °C and 55% RH for 230 days. The RH within the 103 chamber was then lowered to 30% for 105 more days. At given times, the chamber was opened 104 and the specimens' weight was measured to monitor their drying. Eventually, all the specimens 105 were completely dried at 105 °C for porosity evaluation.

### 106 2.3. Permeability assessment (inverse analysis)

107 The intrinsic permeability of the concrete was evaluated using inverse analysis [38–40]. Water

108 transport in unsaturated concrete was described making use of a simplified approach

109 accounting for liquid water permeation only. The contribution of other motions (gas phase

110 permeation and diffusion of vapor) was neglected [38]. Finally, the only differential equation to

111 solve was the following [41,42]:

$$\phi\left(\frac{\partial S}{\partial P}\right)\frac{\partial P}{\partial t} = \operatorname{div}\left[\frac{Kk_r}{\eta}\operatorname{grad}(P)\right]$$
(1)

#### 112 with:

- 113  $\phi$  the concrete porosity (without unit)
- *S* the saturation degree of the porosity (without unit)
- *P* the water pressure within the pores (Pa)

- 116  $\eta$  the water viscosity (Pa s)
- *K* the intrinsic permeability (m<sup>2</sup>)
- 118  $k_r$  the relative permeability to water (without unit)
- 119 The equation proposed by van Genuchten [43] was used to describe the water retention curve:

$$S = \left[1 + \left(\frac{P}{P_0}\right)^{\frac{1}{1-m}}\right]^{-m}$$
(2)

- 120 where m and  $P_0$  are two positive parameters that were identified using the experimental
- $121 \qquad desorption \ isotherm \ measured \ at \ 20^\circ C \ at \ IETcc \ [31]. \ The \ following \ resulting \ values \ were$
- 122 obtained: m = 0.532 and  $P_0 = 59.05$  MPa. It must be mentioned that the fieldcrete desorption
- isotherm was not measured and that a unique dataset was considered here: *i.e.* the desorption

124 isotherm was assumed to be the same for the labcrete and for the fieldcrete. Fieldcretes are

- 125 known to present more variability than labcretes [44]. Using fieldcrete specimens from different
- 126 batches was then expected to possibly induce modifications in their desorption isotherm
- 127 [44,45]. It should also be quoted that using different isotherm data for the labcrete and the
- 128 fieldcrete might have yielded (slightly) different results in permeability [42]; however,
- 129 considering variable isotherm curves was deemed unreasonable due to the number of tests that
- 130 should have been conducted to characterize the desorption isotherm of all the specimens and
- 131 the considerable time that would have been required.
- Following the proposition of Savage and Janssen [46], Mualem's model [43,47] was used to assess the relative permeability to water  $k_r$ :

$$k_{r} = \left[1 + \left(\frac{P}{P_{0}}\right)^{\frac{1}{1-m}}\right]^{-m\alpha} \left\{1 - \left(\frac{P}{P_{0}}\right)^{-\frac{m}{1-m}} \left[1 + \left(\frac{P}{P_{0}}\right)^{\frac{1}{1-m}}\right]^{-m}\right\}^{2}$$
(3)

134 where  $\alpha$  is the pore-interaction factor. It is a lumped parameter that accounts for the 135 connectivity and tortuosity of the pore network. Mualem [47] suggested to use  $\alpha = +0.5$  as 136 default value and so it has been extensively used so far. It was however shown that using

- 137  $\alpha = +0.5$  could sometimes result in inacceptable fits [48] and that  $\alpha$  could exhibit very different 138 values either positive or negative [49,50].
- 139 The left-hand term of eq. (1) was easily obtained by derivation of eq. (2):

$$\phi\left(\frac{\partial S}{\partial P}\right) = -\frac{m\phi}{(m-1)P_0} \left(\frac{P}{P_0}\right)^{\frac{m}{1-m}} \left[1 + \left(\frac{P}{P_0}\right)^{\frac{1}{1-m}}\right]^{-1-m}$$
(4)

140 In practice, eq. (1) was solved using the finite-element method and the code Cast3m<sup>3</sup>. In 141 accordance with the symmetry of the problem, the mesh only accounted for a sample quarter in 142 axisymmetric conditions (Figure 1): 75×150 four-node quadrangles were used in a non-uniform 143 grid. The initial conditions were uniform temperature  $T_{\theta} = 298.15$  K (25 °C) and water pressure  $P_0 = 0.0$  MPa (the samples were initially saturated). The boundary conditions were (for time  $t \ge 100$ 144 0): T = 298.15 K and P = -82.1 MPa for the 230 first days (55% RH) and then P = -165.3 MPa for 145 146 the rest of the simulation (30% RH). Please note that Kelvin's equation (5) was used to calculate 147 the water pressure *P* generated by the relative humidity *h*:

$$P = \rho \frac{RT_0}{M} ln(h) \tag{5}$$

148 with:

• *R* the universal gas constant (8.3145 J/mol/K)

150 •  $\rho$  and *M* the water density (997.1 kg/m<sup>3</sup>) and molar mass (0.018 kg/mol) respectively

151 The intrinsic permeability *K* was then evaluated through the minimization of the quadratic

152 difference between the computed and measured mass variations:

$$F = \sum_{j=1}^{N} \left[ \left( \frac{\Delta m}{m} \right)_{j}^{exp} - \left( \frac{\Delta m}{m} \right)_{j}^{sim} \right]^{2}$$
(6)

153 with:

<sup>&</sup>lt;sup>3</sup> http://www-cast3m.cea.fr/

- *N* the number of mass measurements during the drying test (23 in our case: 12 at 55%)
- 155
   RH and 11 at 30% RH, see Figure 2)
- 156  $\left(\frac{\Delta m}{m}\right)_{i}^{exp}$  and  $\left(\frac{\Delta m}{m}\right)_{i}^{sim}$  the experimental and simulated mass loss for the measurement *j*,

157 see eq. (7)





Figure 1 – schematic description of the mesh and boundary conditions

## 160 3. Results

### 161 3.1. Density and porosity

162 Table 2 presents the density and porosity results. It is interesting to note that the porosity of the 163 fieldcrete (11.9%) was greater than that of the labcrete (10.6%). This was consistent with the 164 density results: the density of the fieldcrete (2.432) was found to be lower than that of the 165 labcrete (2.472). Moreover the intrinsic permeability of the fieldcrete was always greater than 166 that of the labcrete, irrespective of the RH-step, and the experimental scatter obtained for the 167 fieldcrete is about seven times greater than that of the labcrete. This was believed to be due to 168 the increased difficulty of the concreting operations on site as well as to the five different 169 batches [44].

170

171

			Dens	sity	Porosity	
Concrete	Batch	Specimen	Individual	Average	Individual	Average
			value	(COV)	value	(COV)
		Ι	2.474		10.6%	
Laborata	1	II	2.469	2.472	10.7%	10.6%
Laberete	1	III	2.471	(0.1%)	10.7%	(0.8%)
		IV	2.472		10.6%	
	1	1-1	2.421		12.1%	
		1-2	2.455		11.6%	
Fieldcrete	2	2-1	2.440		11.6%	
		2-2	2.439		12.0%	
	3	3-1	2.439	2.432	11.6%	11.9%
		3-2	2.404	(0.6%)	12.3%	(6.5%)
	4	4-1	2.440		11.8%	
		4-2	2.444		11.6%	
	-	5-1	2.419		12.4%	
	5	5-2	2.417		12.2%	

### 174 3.2. Isothermal drying test

175 Figure 2 presents the variations of the specimens' mass loss versus time all along the drying

176 experiment. The experimental mass loss  $\left(\frac{\Delta m}{m}\right)$  was calculated for each specimen as follows:

$$\left(\frac{\Delta m}{m}\right)(t) = \frac{m(0) - m(t)}{m(0)}\tag{7}$$

177 where m(0) and m(t) are the initial mass of the specimen and the mass at time *t* respectively.

178 It is interesting to note that the fieldcrete behaved differently compared to the labcrete: the

179 mass loss was always significantly greater (in line with the porosity that was higher) as well as

180 the discrepancy. Here again, the five different batches as well as the difficulty of the concreting

181 operations onsite may be held responsible.



Figure 2 – mass loss variation versus time

### 184 3.3. Permeability assessment

185 In a first step, the intrinsic permeability was evaluated using inverse analysis independently on 186 the two RH steps (55% and then 30%). The process detailed in section 2.3 was applied to all the 187 specimens. Following Mualem's suggestion [47] and without relevant information about its 188 value, the pore-interaction factor  $\alpha$  was taken equal to +0.5 (1<sup>st</sup> run, Table 3). Separate 189 simulations were conducted for each specimen considering individual data, namely density, 190 porosity and mass loss (Table 2). The permeability assessment was done in two consecutive 191 steps. Firstly, the process detailed in section 2.3 was used to assess the permeability of all the 192 specimens using the results of the first drying phase only (55% RH). In a second step, the results 193 of the second drying phase (30% RH) were used in the same way to assess the permeability of 194 all the specimens once again. In that case, the permeability was assumed to be a piecewise 195 function of time (cf. Figure 3): during the first 230 days (first drying phase at 55% RH) the 196 permeability was fixed to the value obtained in the first simulation and after that the 197 permeability value was adjusted to reproduce the experimental mass variations during the 198 second drying phase (30% RH).



200

Figure 3 – RH and permeability for the 1<sup>st</sup> run of drying simulations

201

202 This approach yielded two different intrinsic permeability values for each specimen: *K*(55%)

203 and *K*(30%) that are presented on Figure 4. The variability obtained for the fieldcrete was

always significantly greater than that of the labcrete (about 4 times) in accordance with the

205 experimental mass loss results (Figure 2).

#### Table 3 - summary of the simulations

Parameters/properties		1 <sup>st</sup> run	2 <sup>nd</sup> run		
Porosity Ø		See the individual values of	See the individual values of		
Density	$d_s$	Table 2	Table 2		
van Genuchten exponent	m	0.532	0.532		
van Genuchten pressure	$P_0$	59.05 MPa	59.05 MPa		
Pore interaction factor	α	+0.5	$\alpha$ and <i>K</i> adjusted together		
		adjusted on the two RH steps	using the results of the two RH		
Intrinsic permeability	K	(30% & 55%) resulting in two	steps (30% & 55%) resulting in		
		distinct values	a unique dataset		

207

208 It is noteworthy that the intrinsic permeability values obtained at 30% RH were higher than

those of 55% RH (by a factor 2-3, see 1<sup>st</sup> run in Table 4). This indicated that the relative

210 permeability  $k_r$  was not correctly estimated and more specifically the slope between 55% and

211 30% RH was overestimated. This was due to the choice of the  $\alpha$  value (+0.5) that did not

properly describe the relative permeability variations of the considered concrete. This is known
to induce significant discrepancy in the assessment of the intrinsic permeability over different
RH ranges [41].



216 In a second step, the pore interaction factor  $\alpha$  was considered as an unknown empirical

217 parameter that needed to be calibrated together with the intrinsic permeability *K* as it is

218 commonly done in soil science [48–53] ( $2^{nd}$  run, Table 3). The value of  $\alpha$  was adjusted so that the

effective permeability (*i.e.* the product  $K \times k_r$ ) matched the two different effective

220 permeabilities assessed at 55% and 30% RH (see the two black spots on Figure 5). The  $\alpha$ -values

thus obtained are reported in Table 4 (column '2<sup>nd</sup> run'). In so doing, it was believed that the

slope of the effective permeability curve was correctly calibrated (at least between 55% and

223 30% RH).



225

Figure 5 – calibration of the pore-interaction factor  $\alpha$  (example of the fieldcrete specimen 1-1)

New simulations of the drying experiments were conducted for all the concrete specimens using the pore interaction factor values that were obtained above. For each specimen a unique value of intrinsic permeability was identified that made it possible to describe the mass loss variation all along the drying experiment (see 2<sup>nd</sup> run in Figure 6). This proved that the pore interaction factor  $\alpha$  was properly evaluated and that the resulting data set could be used to describe accurately the water exchange with the environment down to 30% RH.



#### **233** Figure 6 – new assessment of the intrinsic permeability K using $\alpha \neq +0.5$ (example of the fieldcrete specimen

1-1)

234

232

235 All the results in terms of permeability and pore interaction factor are reported in Table 4 and 236 plotted in Figure 7. It is interesting to note that after the second assessment step, the intrinsic 237 permeability values obtained for the fieldcrete were very close to those of the labcrete (Figure 238 8). This was not the case after the first step. Reevaluating the pore interaction then helped to 239 improve the accuracy of the evaluation and eventually show that the labcrete and fieldcrete 240 were very similar in terms of intrinsic permeability  $(2 \times 10^{-22} \text{ m}^2)$ . The reader must keep in mind 241 though that the intrinsic permeability assessed using inverse analysis depends on the model and 242 input data used [42]. One can wonder whether the conclusion would have been the same using a 243 different evaluation process.

All the pore interaction factors presented negative values that were different for the labcrete and fieldcrete: they ranged between -0.5 to -0.6 for the labcrete and between -1.0 to -1.4 for the fieldcrete. It is noteworthy that all these values were different from the value suggested by Mualem (+0.5). This has been known for long for soils for which many results were published [47–50,53–55]. In the field of cement-based materials, results are scarce. A positive value of +5.5 was proposed using gas permeability tests [2,56] but negative values were obtained by Leech et al. [57] using capillary absorption tests: they obtained values ranging from -0.2 to -1.2. Later

251	Poyet <i>et al.</i> [41] dried partially carbonated specimens with decreasing RH steps and after
252	inverse analysis obtained values ranging from -1.5 to -4.0. It is interesting to note that the values
253	obtained in this study for the labcrete matched the proposition of Leech <i>et al</i> . to use $\alpha = -0.5$
254	instead of +0.5 [57]. The $\alpha$ -values of the fieldcrete were somewhat lower (-1.2 in average).
255	In terms of experimental scatter, the variability of the intrinsic permeability of the labcrete was
256	very low: the coefficient of variation was 3%. This was expected because all the four specimens
257	were carefully fabricated in the laboratory using the same concrete batch. The coefficient of
258	variation of the fieldcrete was found to be higher (12%) because the specimens originated from
259	five different concrete batches that were fabricated onsite by the workers in charge of the
260	realization of the surface disposal mockup. The coefficient of variation that was found for the
261	fieldcrete however remained limited compared to the values obtained in other studies – see for
262	instance [44] - indicating that it is possible to limit the variability of concretes in situ.

~	-	
2	6	Δ
_	υ	т

Table 4 – intrinsic permeability and pore interaction factor da	ta

Comercete	Datah	Succimon	1 <sup>st</sup> run			2 <sup>nd</sup> run	
concrete	Batch	Specimen -	α	<i>K</i> (55% RH)	K(30% RH)	α	K
		Ι	+0.5	3.3×10 <sup>-22</sup>	6.2×10 <sup>-22</sup>	-0.49	2.2×10 <sup>-22</sup>
Laborata	1	II	+0.5	3.2×10-22	6.2×10 <sup>-22</sup>	-0.54	2.1×10 <sup>-22</sup>
Laberete	1	III	+0.5	3.5×10-22	7.2×10 <sup>-22</sup>	-0.63	2.2×10-22
		IV	+0.5	3.4×10-22	6.8×10 <sup>-22</sup>	-0.59	2.2×10-22
Fieldcrete	1	1-1	+0.5	3.6×10-22	9.4×10 <sup>-22</sup>	-1.00	2.3×10-22
		1-2	+0.5	2.7×10-22	7.1×10 <sup>-22</sup>	-1.02	1.7×10-22
	2	2-1	+0.5	3.5×10-22	11.0×10 <sup>-22</sup>	-1.30	1.6×10 <sup>-22</sup>
		2-2	+0.5	3.7×10-22	11.3×10 <sup>-22</sup>	-1.25	2.2×10-22
	3	3-1	+0.5	3.4×10 <sup>-22</sup>	9.3×10 <sup>-22</sup>	-1.08	2.1×10 <sup>-22</sup>
		3-2	+0.5	4.5×10-22	15.2×10 <sup>-22</sup>	-1.41	2.6×10 <sup>-22</sup>
	4	4-1	+0.5	3.3×10-22	9.8×10 <sup>-22</sup>	-1.21	1.9×10 <sup>-22</sup>
		4-2	+0.5	3.6×10 <sup>-22</sup>	10.9×10 <sup>-22</sup>	-1.24	2.1×10 <sup>-22</sup>
	5	5-1	+0.5	4.7×10 <sup>-22</sup>	13.5×10 <sup>-22</sup>	-1.15	2.7×10 <sup>-22</sup>
		5-2	+0.5	3.9×10 <sup>-22</sup>	12.9×10 <sup>-22</sup>	-1.38	2.2×10-22





267 Figure 8(a) compares the unsaturated permeability evolutions for all the tested specimens. 268 Although the intrinsic permeability values (S=1) were more or less the same for the laborete and 269 the fieldcrete, the fieldcrete specimens were always more permeable than the labcrete ones. At 270 55% RH (*S*=0.555), the effective permeability of the fieldcrete was between once and twice that 271 of the labcrete. At 30% RH (S=0.293), the effective permeability of the fieldcrete was between 272 1.4 and 3.4 times that of the labcrete (Figure 8(b)). This was due to the differences in pore-273 interaction factor  $\alpha$  (Figure 7) that influenced the slope of the effective permeability. It is 274 noticeable that, below 30% RH, the fieldcrete permeability steeply increased faster than that of 275 the labcrete when saturation decreased. The fieldcrete permeability could then be ten times 276 higher than that of the labcrete for very low saturation values. However this point was not 277 judged significant for two reasons. Firstly, it must be recalled that this increase was obtained for 278 RH values that were much lower than 30%; these values are almost never encountered in real 279 life. Secondly, the increase was obtained for saturation values that were very far from the RH-280 domain in which the permeability was evaluated. This increase might then be somewhat 281 questionable.



## 284 4. Application: simulations of drying

#### 4.1. 1D simulation of a homogeneous material

286 To illustrate the effects of the identification procedure on the saturation degree profiles, we 287 propose to simulate in this section the case of a homogeneous material subjected to drying at 288 constant relative humidity. The parameters identified in the previous section will be 289 successively adopted and the obtained results will be compared. The structure considered 290 consists of a fraction of concrete wall with thickness 20 cm, and with its two opposite faces 291 exposed to a relative humidity of 55% (see Figure 9). The drying phenomenon is assumed to 292 occur perpendicularly to these faces and is one-dimensional, though the resolution of the 293 problem is 2D. For symmetry reason, only half of the structure is considered. Again, the finite 294 element code Cast3m is used to solve eq. (1), with 400 elements having variable dimensions 295 (their size is smaller near the exposed surface to capture accurately the high gradients 296 appearing when the loading is applied, and increases progressively) to discretize the structure.



Figure 9 – schematic description of the 1D simulations and boundary conditions

300 The first simulation is intended to compare the results of labcrete and fieldcrete corresponding to the identification procedure with  $\alpha \neq 0.5$  shown in Figure 7, *i.e.* for the mean values of 301 302 parameters for both materials. Note that the respective average value of porosity (see Table 2) is 303 used for each case. The saturation degree profiles obtained at 100 days, 1 year and 3 years of 304 drying are plotted in Figure 10 as a function of the depth, x=0 designating the exposed face. Very 305 few differences can be observed between labcrete and fieldcrete profiles, indicating that on 306 average the two materials exhibit similar drying processes and then close permeability 307 properties in unsaturated conditions.







312 We now examine the influence of the permeability value retained for the identification (i.e., at 30 313 and 55% HR, see Figure 5 and Table 4, 1<sup>st</sup> run) on the description of the drying kinetics when the 314 parameter  $\alpha$  is kept equal to 0.5. Figure 11 presents the saturation profiles obtained at 100 days 315 and 3 years in the case of fieldcrete 1.2 and 3.2, and for the two values *K*(55%) and *K*(30%). 316 These cases are chosen because they appear to envelop all curves with the  $\alpha = -1.2$ 317 identification procedure (see Figure 12). For the sake of comparison, we also reported in dotted 318 lines the curves simulated with  $\alpha = -1.2$  and shown on Figure 10.



Figure 11 – saturation profiles at 100 days and 3 years for fieldcrete 1.2 and 3.2 obtained with parameters  $\alpha = 0.5$  and two values of permeability; comparison with the identification of Figure 7 ( $\alpha = -1.2$ )

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We first observe that the saturation profiles simulated with the two permeability values exhibit very significant differences. Further, the *K*(55%) curves are at the same time close to each other and close to the  $\alpha = -1.2$  average case. This is not very surprising since the validity domain of the parameters identified at 55% is more consistent with the practical RH domain covered in the simulation than the one identified at 30%. Finally, we conclude that the *K*(55%) with  $\alpha = 0.5$ values provide saturation profiles in good concordance with those obtained with the  $\alpha = -1.2$ identification method.

Figure 12 presents the saturation profiles obtained at 100 days, 1 year and 3 years for all labcrete (top) and fieldcrete (bottom) specimens calculated with the parameters of the 2<sup>nd</sup> run of Table 4 corresponding to  $\alpha \neq 0.5$ . We observe that for labcrete, the curves are relatively close whatever the samples considered, while for fieldcrete the scatter is as expected much more significant. Although we may argue that the greater number of fieldcrete specimens also
contributes to this larger variability, the more disperse response for these concrete samples
appears clearly and leads to important differences in saturation profiles.



specimens calculated with the parameters of the 2<sup>nd</sup> run of Table 4

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These results are totally in line with those shown on Figure 2 and Figure 8. The discrepancies in the saturation degree profiles increase as a function of time (at least up to 3 years), which means that the time needed for obtaining a quasi-homogeneous saturation profile may differ 347 considerably in particular between the fieldcrete specimens. As a corollary, the question of the 348 notion of representative elementary volume is posed as it may not to be the same for labcrete 349 and fieldcrete, *i.e.* a greater volume is expected for fieldcrete to appropriately represent the 350 material with a variability similar to the labcrete one.

Among the possible causes of the greater variability in the fieldcrete results, a more significant dispersion in the spatial repartition of the different components (aggregates, cement paste, pores) due to a lower homogeneity in the casting procedure, and the variability in the actual formulation, are expected to be of importance. We propose to examine the first aspect in the next section through simulations of mesoscale concrete specimens exhibiting a different aggregate distribution.

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### 4.2. Simulation of 3D concrete samples

359 To investigate the role of the aggregates within the specimens on the overall drying kinetics, we 360 propose to perform mesoscale 3D simulations on numerical samples generated with different 361 aggregate distributions and shapes. Such mesoscale simulations on concrete representative 362 volumes involving explicitly the aggregates are increasingly used due to the growing power of 363 computers to analyze various effects and characterize properties related to (possibly coupled) 364 mechanical, diffusive and chemical problems, see for instance [58-61] In this paper, to be as 365 close as possible to the experimental conditions of fieldcrete testing, the numerical samples are 366 constructed following the experimental procedure, *i.e.* cubic concrete volumes with dimensions 367 15×15×15 cm are generated, from which cylindrical samples of diameter 6 cm and height 11 cm 368 are extracted (cored). The aggregate dimensions are imposed by the actual grading curve. Note 369 that the aggregates are generated numerically with convex polyhedral shapes obtained by a 370 Voronoi space decomposition, which is a notable difference with e.g. [61] in which aggregates 371 are spherical. The aggregates are next modified to conform to a prescribed aspect ratio 372 randomly chosen between 1 and 4 along two perpendicular directions, so as to generate

373 flattened/elongated shapes. The numerical procedure makes use of the functionalities of the 374 CAD code Salome (www.salome-platform.org), and is described in more details in *e.g.* [62–64]. 375 Although these numerical aggregates are expected to be relatively realistic, the obtained 376 approximated shapes (in particular, real aggregates are not in general convex) may introduce a 377 certain bias in the results. However it has been reported in [65] that regarding viscoplastic mechanical behavior, such numerical aggregates reproduce relatively well the overall concrete 378 379 behavior when compared to real aggregates obtained by tomography. A similar study regarding 380 transport properties would be necessary to investigate the impact of real versus numerical 381 aggregates.

382 Figure 13 left presents a generated cubic specimen with 12370 aggregates (left), corresponding 383 to an aggregate volume fraction of 35% and a minimum size on the grading curve of 3.6 mm. 384 Such ratio is deemed to be sufficiently realistic to achieve representative results, while keeping 385 the computation costs reasonable. Note that the random process of particle placing accounts for 386 a minimum distance between aggregates, and has to fulfill the non-overlapping condition with 387 the cube surfaces. Figure 13 right shows the aggregate distribution in 3 cylindrical specimens 388 cored from different cubic samples. For the simulations, 6 samples have been extracted from 3 389 different cubes. Interestingly, the aggregate volume fraction calculated in the specimens ranges 390 between 0.374 and 0.383, which is significantly higher than the one imposed in the initial cubic 391 volumes due to the wall-effect and corresponding non-homogeneity of the aggregates 392 repartition in the cubes between regions near the surfaces and the core.





Figure 13 – example of 15×15×15 cubic specimen generated with 12370 aggregates (left); aggregate distribution in 3 cylindrical specimens constructed from the cubic samples (right)

396 The meshes are generated automatically by the meshing softwares MG-CADSurf and MG-Tetra 397 developed by Distene<sup>4</sup>, and plugged in Salome. The total number of tetrahedral elements in the 398 meshes of the cylindrical specimens range between 2.26 and  $2.32 \times 10^6$ . The simulations consist 399 of a drying test from an initial totally saturated state during 1 year, and with the lateral surfaces 400 of the specimens exposed to an environment with RH = 0.55. To focus on the aggregate shape 401 effects and ease the comparison, the material parameters of the matrix phase (corresponding 402 here to the mortar) are supposed to be the same for all samples, and are taken as  $K=2\times10^{-22}$  m<sup>2</sup>, 403  $\alpha = -0.56$ , and  $\phi = 0.2$ . Note that as the values of K and  $\alpha$  are not identified experimentally on 404 mortars, they are simply set from those determined for concretes in the previous sections, given 405 that we do not expect that the results regarding the effects of aggregate shapes would be 406 different with (slightly) altered values. The macroscopic transport properties obtained on the 407 numerical specimens with these values for mortar are calculated and discussed in the sequel. 408 The aggregates are not accounted for in the calculations since they are supposed to be non-409 diffusive. Also, the possible preferential pathways for transport at the interfaces between 410 aggregates and matrix (the so-called ITZ) are ignored here. Indeed, we assume that, as by

<sup>&</sup>lt;sup>4</sup> http://www.distene.com

411 construction these interfaces do not form a connected network, their impact on the overall412 results is weak.

413 Figure 14 presents the simulation results in terms of time evolution of overall saturation degree 414 (left) and water mass (right) calculated within all 6 specimens. The mass of water is simply 415 obtained from the saturation degree and the average porosity in the whole samples, *i.e.* the 416 porosity corrected by the volume fraction of matrix. We can observe that the saturation degree 417 curves are identical for all cases, while the water mass ones exhibit a slight difference. The latter 418 are mainly attributed to the different mean porosity in the samples, which is a consequence of 419 the variable volume fraction of matrix due to the random generation process of the numerical 420 samples. From these results, we may assert that, on average, the global drying response is nearly 421 the same for the specimens. This indicates that regarding the saturation degree averaged over 422 the entire volume, the influence of the aggregate distribution as investigated in this section is 423 negligible.







429 As mentioned above, it may be instructive to characterize the macroscopic (or equivalent) 430 transport parameters of the generated numerical concretes, from the results of water mass loss 431 of Figure 14 as done in section 3 from experiments, and to compare them with the input data of 432 mortar. Assuming the same value of  $\alpha$  for both materials, *i.e.*  $\alpha = -0.56$ , we then propose to 433 apply the inverse analysis procedure described above to identify the permeability coefficient. 434 Figure 15 presents the curves obtained on a homogeneous cylinder of diameter 6 cm and height 435 11 cm with different values of K (continuous lines), and the mean curve resulting from the 3D 436 numerical simulations on the 6 reconstructed specimens (points). The comparison indicates that 437 the value  $K=0.75\times10^{-22}$  m<sup>2</sup> leads to a water mass loss kinetics very close to the numerical 438 concrete one. This means that the hypothesis on the value of  $\alpha = -0.56$  is relevant for the 439 homogenous material; on the other hand, the permeability coefficient K is significantly lower 440 than the one of the mortar.



441

442 Figure 15 – evaluation of the average permeability of the 6 reconstructed 3D specimens using inverse 443 analysis (they were considered as homogeneous materials)

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It is important to notice that while the identification procedure is performed on a material assumed as homogeneous, hence with its entire boundary surfaces exposed to drying, the exchange of water takes place only through the contact surfaces between mortar and atmosphere in the 3D simulations, since the aggregates that overlap the lateral surfaces are nondiffusive. This means that the surface exposed to drying is much lower in the latter case than in the former one, which may according to the authors explain at least partly the important difference between macroscopically identified permeability coefficient and the prescribed input 452 data set for the mortar. Indeed, it is doubtful that that the dilution effect and tortuosity due to 453 the presence of aggregates, which represent about 40% of the volume in the generated 454 specimens, may be totally responsible for a permeability coefficient decrease by a factor of 2.7. 455 To be more directly comparable, the value for mortar should also be affected by the reduction of 456 drying surface. As a first approximation, if we simply consider the same ratio for the surface 457 available for exchange and the volume fraction of mortar in concrete, *i.e.* around 60%, and that 458 this ratio may be directly applied for estimating the 'homogenized' mortar permeability in the 459 homogenous concrete, we arrive at a value of  $K \approx 1.2 \times 10^{-22}$  m<sup>2</sup> instead of  $K = 2 \times 10^{-22}$  m<sup>2</sup>, which 460 seems in better agreement with the macroscopic value of  $0.75 \times 10^{-22}$  m<sup>2</sup>. This aspect would 461 however deserve further investigation.

462 To investigate in more details the numerical results on the 3D specimens, Figure 16 shows the 463 saturation degree profiles in the 6 samples at 5 days, 100 days and 1 year. The horizontal axis 464 designates the radius of the specimens, with 0 being the center and 0.03 the external surface. 465 The curves are obtained by averaging the calculated saturation degree fields on cylindrical 466 surfaces whose axis is identical to the samples one and whose radius evolves progressively from 467 0 to 0.03. Compared to Figure 14 showing volume-averaged quantities, Figure 16 then presents 468 surface-averaged results, which are deemed to provide more insightful and accurate information 469 about the aggregate distribution effects. We observe however that the curves for the different 470 specimens cannot be really distinguished; only a very small discrepancy may be seen on the 100 471 days results. This means that, in line with the conclusion on Figure 14, the saturation degree 472 profiles are not significantly affected by the aggregate distribution as considered here.

Finally, Figure 17 presents the numerical results in a more local manner than the two previous Figures, with the saturation degree averaged over circles centered on the specimen axis. The procedure is basically similar to the one leading to Figure 16, except that the cylindrical surfaces of interest are here sampled by plans perpendicular to the axis. The idea is to examine the evolution of the saturation degree along the axial direction at prescribed distances from the 478 surface exposed to drying, and at different times. We propose to analyze the results near the 479 lateral surface at the radius r = 0.027 m, and also at mid-distance between the axis and the 480 surface at the radius r = 0.015 m, corresponding to Figure 17 top and bottom, respectively, and 481 at 5, 25 and 100 days. The abscissa designates the position of the points along the axis, with 0 482 being arbitrarily the lower cross-section of the specimens. We observe that the results at 483 r = 0.027 (top) exhibit non-negligible variations along the axis direction, but also between the 484 different specimens. This is particularly visible at the onset of drying (5 days), while the curves 485 tend progressively to homogenize at greater times, with differences becoming relatively weak at 486 100 days. Maximum discrepancies of about 4.5% and 2.5% are reported at 5 days and 100 days, 487 respectively. The results at r = 0.015 show an opposite tendency: from the initial prescribed 488 homogeneous state, the saturation degree turns out to gradually disperse for increasing times, 489 though moderately; at 100 days, the maximum difference between all results is less than 3%.

To sum up, the curves of Figure 17 indicate that the aggregates influence locally the drying phenomenon all the more that the gradients of saturation degree (or equivalently of capillary pressure) are high, *i.e.* the kinetics of transport is rapid. At the beginning of the simulations these gradient are maximal near the exposed surfaces, and the presence of aggregates as obstacles to water transfer is noticeable. By contrast, when gradients are low as in the specimen centers or at greater times, their influence and correspondingly their size and shape distribution, become more and more negligible.



499 Figure 16 – saturation degree profiles as a function of the radius for the 6 calculated specimens at 3 different 500

498

times

501 To conclude with the 3D numerical simulations presented in this subsection, the spatial 502 distribution of aggregates within the samples seem to have a limited impact on the drying 503 characteristics. When examining saturation degree evolutions as volume- and surface- averaged 504 quantities, this aspect is clearly negligible. Locally, the influence of aggregates is visible in the 505 zones where the gradients of capillary pressures are high, *i.e.* essentially at the beginning of 506 drying near the exposed surfaces. Note that in practice, due to cyclic and seasonal environmental 507 conditions, significant gradients may persist in these zones, meaning that the involved 508 aggregates may have a certain impact on the kinetics.



512 Figure 17 – saturation degree profiles as a function of the radius for the 6 calculated specimens at 3 different

times.

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514 Overall, considering all the other factors as constant, the variability in the (coarse) aggregate 515 distribution as investigated here cannot explain the dispersion observed experimentally in the 516 fieldcrete (and also to a lesser extent in the labcrete) specimens. Some other reasons should be 517 pointed out, as the variability in the formulation and in the phase properties of the cement paste. 518 To be addressed, these aspects would need to be characterized experimentally, which 519 constitutes a challenging aspect.

520

## 521 5. Conclusion

522 In order to characterize the difference in permeability between labcrete and fieldcrete, the 523 unsaturated permeability to water of a modern concrete was evaluated using inverse analysis. 524 Labcrete specimens were prepared and cured in the laboratory and fieldcrete specimens were 525 prepared during the construction of test panels (ca 25m<sup>3</sup>). The fieldcrete appeared to be more 526 porous than the labcrete (11.9% in average vs. 10.6%) but, using inverse analysis and 527 accounting for water permeation only, the intrinsic permeability values were very close for the two concretes  $(2.2 \times 10^{-22} \text{ and } 2.1 \times 10^{-22} \text{ in average for the labcrete and fieldcrete, respectively}).$ 528 529 The fieldcrete however exhibited lower pore-interaction factor (*i.e.* the parameter of Mualem's 530 model that accounts for pore structure tortuosity and connectivity) than the labcrete (-1.2 vs. -531 0.56), indicating that the tortuosity and connectivity of the poral network were not the same for 532 the two concretes. The fieldcrete also displayed more scatter, which can be mainly attributed to 533 the five distinct batches that were considered. Clearly enough, non-negligible discrepancies were 534 reported in the identified relative permeabilities for the two concretes, in particular for 535 saturation degrees below about 0.7. These differences increased for decreasing values of 536 saturation, the relative permeability of fieldcrete remaining higher. This means that the drying 537 kinetics of fieldcrete would be potentially faster for low saturation, but in practical 538 environmental conditions such small saturation states are likely to be rarely met. 539 Moreover, one-dimensional simulations performed on a saturated homogeneous concrete wall 540 subjected to drying at HR=55% showed very little differences between fieldcrete and labcrete 541 (with model parameters prescribed as the averaged ones) in terms of saturation degree profiles 542 at various times. By contrast, important variations were observed when the parameters 543 identified on the various fieldcrete specimens were successively considered in the calculations. 544 Finally, as a first attempt to investigate the effects of the aggregate distribution on the variability 545 observed on the experimental results, 3D mesoscale simulations were carried out on 546 reconstructed cylindrical specimens of same dimensions as the tested ones. Only the aggregate

547 distributions and shapes were varied between the 3 generated cubes where the 6 samples were 548 cored. This resulted in slight variations of aggregate volume fraction between the specimens. 549 Overall, the main results indicated that the evolutions of volume-averaged saturation degrees 550 and surface-averaged saturation degree profiles were almost identical for all 6 specimens. Only 551 by examining the saturation degree at given distances from the exposed surface along the axis 552 direction of the samples can be observed non-negligible variations, in particular near the surface 553 where the saturation gradients are higher. This means that the different aggregate distributions 554 between numerical specimens lead to significant local saturation disparities, but cannot alone 555 explain the observed macroscopic variability. An important part may originate from the matrix 556 properties themselves (*i.e.* spatial variability in the content, the porosity, the placement etc.), 557 which are however quite difficult to characterize experimentally. This aspect would deserve to

558 be addressed, both on the numerical and experimental grounds.

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