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# 1 Development of a micro-mechanical model for 2 the determination of damage properties of 3 cement pastes

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10

## 11 Abstract

12

13 Demand on low-carbon concrete for building increases in many countries. However, workers  
14 in construction sites are often confronted with early cracking risks in concrete when new  
15 cement mixtures are used. Indeed, new chemical additions are mixed with cement and  
16 mixtures are optimized in laboratories to reach the target performance for concrete. But, in  
17 site, the results are not exactly the same. In order to help concrete suppliers design new low-  
18 carbon concrete, it is necessary to control the cracking risk of concrete. To consider all  
19 phenomena into concrete, a modelling approach starting at the micro-scale seems to be the  
20 best tool for the prediction of any concrete mixture in any environment. A numerical protocol  
21 at the micro-scale is proposed in order to determine the damage properties of cement pastes.  
22 The method is based on a once-for-all calibration of parameters which remain unchanged for  
23 any other mixtures. Validations were made using tensile and compressive tests on different  
24 cement pastes. The numerical results are in good agreement with experimental data of four  
25 cement pastes with different water-to-cement ratios and mineral additions, and of six mixtures  
26 obtained from the literature. The results demonstrate the predictive power of the numerical  
27 approach and its utility for a quick assessment of material properties.

28

## 29 Keywords

30 Cement pastes; Micro-mechanics; Damage; Finite element model

31

## 32 **1 Introduction**

33 This study aims to give a decision-making tool to concrete suppliers to design new low-  
34 carbon concretes. Many customers ask for high performance concrete structures with low  
35 cement content by replacing it with mineral additions (fly ash, slag, etc.) [1–3]. But, workers  
36 in construction sites observe more cracking in new concretes than in classical concretes. The  
37 links between cracking in these new concretes with environmental conditions and casting  
38 methods are not totally clear. Concrete suppliers assess the strength of concrete in  
39 laboratories, albeit under controlled conditions. In addition to that, only statistical evaluations  
40 can be done by linking the influence of one component on the global behaviour. New concrete  
41 mixtures need to define the properties of the new cement paste by performing numerous tests.  
42 In order to limit the tests, many researchers have given elastic properties of the concrete  
43 components to link the global behaviour to the mixture. These properties, obtained by nano-  
44 indentation measurements, were also used in models and gave good results in comparison with  
45 elastic tests. However, under inelastic loading, these models used empirical parameters for  
46 fracture properties [4–8]. So, for new concrete mixtures, new adjustments are necessary. It is  
47 thus unpractical to use the previous approach to understand the influence of environmental  
48 conditions and casting methods under non-controlled conditions, as in construction sites.

49 On another note, in order to correctly predict the durability of low-carbon concrete structures,  
50 multi-physics models need to use physical properties reflecting real processes. It seems  
51 therefore important to consider damage properties not dependant on the mixture and test  
52 conditions to predict damage of a variety of cementitious materials [9–11].

53 It is very difficult to consider all the details of the cement paste's microstructure in a unique  
54 volume for modelling without undermining the computation time. Indeed, two scales can be  
55 considered: a molecular scale ( $10^{-8}$  to  $10^{-6}$  m) [12–15] and a microscopic scale ( $10^{-6}$  to  $10^{-4}$   
56 m). The first is used to calculate the intrinsic properties of the components independently of  
57 the hydration or loading. The second considers an assembly of the last components, obtained  
58 by cement hydration, with properties that are linked to the properties obtained by the first  
59 method, or found via experimental measurements.

60 In this respect, a representative elementary volume (REV) is defined to represent the cement  
61 paste. The REV should be small enough to consider all the components in an explicit manner,  
62 and big enough to represent a macroscopic sample of the heterogeneous material. A size of  
63  $100\ \mu\text{m}$  is often used by authors [16–21]. Others, however, suggest smaller [22,23] or bigger  
64 sizes [17,24], in the range of  $50\ \mu\text{m}$  to  $400\ \mu\text{m}$ . The choice of the REV is made according to

65 the size of the biggest inclusion, usually five times the diameter of the largest inclusion [25].  
66 The simulations start with the generation of a virtual microstructure of the cement paste  
67 whose phase assemblage mimics the real distribution and composition of phases in the real  
68 microstructure. This can be achieved by means of numerical hydration models. Several codes  
69 and tools have been developed for this, and a review of the available hydration models can be  
70 found in Thomas et al. [26].

71 In the present study, the Virtual Cement and Concrete Testing Laboratory (VCCTL) platform  
72 [24] has been chosen for the cement paste's microstructure generation. This programme,  
73 which is based on the cellular architecture of CEMHYD3D [27,28], allows for an explicit  
74 representation of the cement phases as well as the incorporation of admixtures such as slag,  
75 fly ash and silica fume. Consequently, a mesh algorithm [29] was used to import the hydrated  
76 cement paste volume in the finite element code Cast3M [30] for mechanical simulations.

77 In this paper, a micro-mechanical approach for the determination of the damage properties of  
78 cement pastes is proposed. The objective of this approach is to avoid the multiple tests for the  
79 characterization and readjustment of the mechanical properties. The elastic properties of the  
80 cement paste's components were founded in the literature. The damage model of Fichant et al.  
81 [31] was chosen for its simplicity and quality to simulate the mechanical damage of cement-  
82 based materials. This damage model is independent of the scale and correctly reproduces the  
83 softening behaviour of a damaged material. A parametric study was performed with the goal  
84 to find the relationship between the damage properties of the cement paste's components.

85 First of all, the numerical method is described in three sections: the cement type chosen and  
86 the virtual representation obtained from VCCTL are presented, the damage model used in the  
87 finite element modelling is given in detail, and the numerical protocol is explained to show  
88 the unknown parameters to identify. Second of all, the numerical results regarding the damage  
89 properties of the cement paste's components are discussed. Finally, simulations for tensile and  
90 compressive tests are compared to experimental data for a wide range of cement types.

## 91 **2 Presentation of the micro-mechanical approach**

### 92 **2.1 Tested materials and virtual cement hydration**

93 A typical Portland cement paste contains about a dozen cement phases. This includes  
94 unhydrated particles with clinker phases and sulfates (gypsum, hemihydrate and anhydrite),  
95 and the products of hydration which mainly contain calcium silicate hydrate (or C-S-H),  
96 portlandite, ettringite and sulfo-aluminates (AFm). The number of phases in composite

97 cements increases sharply in the presence and the hydration of slags, fly ash, silica fume,  
98 fillers and other minor phases. The gradual formation of hydrates and their distribution within  
99 the matrix provide the cement paste with increasing cohesion, stiffness and strength.

100 The mineral compositions of the cements incorporated in the VCCTL model are listed in  
101 Table 1. The composition of Portland cements, labelled CEM-N1 and -N2, were obtained  
102 from their technical files while the data for the remaining cements are extracted from the  
103 “CemBase” database compiled by the Nanocem consortium [32,33]. These cement paste  
104 compositions that are considered in micro-mechanical simulations are divided into three sets:

- 105 ➤ The first set consists of only one cement paste, labelled CP1-0.45, used as a reference  
106 point for the identification of failure properties of cement paste phases. This cement paste  
107 is made from ordinary Portland cement (CEM-N1) with a water-to-binder ratio of 0.45.
- 108 ➤ The second set consists of three cement pastes used for the testing of the model on other  
109 compositions. Two of these cement pastes are made from CEM-N1 with w/b= 0.4 and 0.5  
110 (labelled CP1-0.4 and CP1-0.5, respectively), while the third is made from CEM-N2 with  
111 w/b=0.45 (labelled CP2-0.45).
- 112 ➤ Using data available from the literature, the third set consists of 23 cement pastes, used  
113 by the model to predict their respective compressive strengths. 18 of these are composed  
114 of other Portland cements (labelled CEM-IA, -IB...-IF) while the remaining five are  
115 made of composite cements with different admixtures (cf. Table 1).

116 It should be noted that cement phases are explicitly represented inside the microstructure  
117 volume, including C-S-H and capillary porosity. The term "phase" is used here in the same  
118 sense used in the hydration model VCCTL. Therefore, the C-S-H gel, which can be  
119 decomposed into low density C-S-H, high density C-S-H and gel porosity [31], is considered  
120 as a single phase and is represented by one voxel type. Water-filled porosity is also counted as  
121 another "phase", regardless of the water content in the capillary voids. A full list of the phases  
122 included in the VCCTL model is available on the programme's online user guide.

123 The representativeness of the REV of the cement paste is controlled by the resolution of the  
124 microstructure voxels ( $1\mu\text{m}^3$ , as imposed by the hydration model) and its size. Taking into  
125 account the grading curve of the cement (99% of particles are smaller than  $60\mu\text{m}$  in size), a  
126  $200\times 200\times 200\mu\text{m}^3$  cube was chosen as REV. The simulation of hydration in VCCTL proceeds  
127 by cycles. A conversion of cycles into units of time would not be necessary if the user is only  
128 interested in the evolution of the degree of hydration (which is the case for the third set of  
129 cement pastes). However, selecting the hydrating microstructure at the exact age of 28 days is  
130 needed to determine the micro-mechanical parameters from experimental results.

**Table 1. Mineral composition of cements used and mix compositions of cement pastes (Values represent mass fractions. Clinker phase fractions are given on a clinker basis).**

Cement Phases Cement pastes		Primary constituents of cement							Secondary constituents					
		Clinker phases							Sulfates	Calcium carbonate	Limestone	Slag	Silica fume	Quartz
Label	w/b (DoH %) ‡	C <sub>3</sub> S	C <sub>2</sub> S	C <sub>3</sub> A* <sup>‡</sup>	C <sub>4</sub> AF	K $\bar{S}$	N $\bar{S}$	CSH <sub>x</sub> <sup>†</sup>						
CEM-N1	0.4 (67.3 %)	72.2	9.4	9.4	7.3	1.3	0.3	4.2	1	1	0	0	0	0
	0.45 (69.7 %)													
	0.5 (76.9 %)													
CEM-N2	0.45 (65.3 %)	69.1	9.1	7.5	11.4	2.8	0.2	1.5	6	2	0	0	0	0
CEM-IA	0.677 (90.2 %)	66.9	8.0	14.1	4.4	0	0	4.6**	0	0	0	0	0	0
	0.497 (84.9 %)													
	0.32 (61.4 %)													
CEM-IB	0.688 (87.4 %)	67.5	7.0	6.0	10.0	0	0	4.6**	0	0	0	0	0	0
	0.505 (82.3 %)													
	0.325 (60.3 %)													
CEM-IC	0.681 (83.6 %)	58.0	18.2	8.0	10.0	0	0	3.2**	0	0	0	0	0	0
	0.503 (79.6 %)													
	0.323 (60 %)													
CEM-ID	0.454 (73.8 %)	63.2	13.3	2.0	12.9	0	0	4.3**	0	0	0	0	0	0
	0.364 (64.7 %)													
	0.274 (55.1 %)													
CEM-IE	0.683 (82.3 %)	54.5	19.2	8.4	9.8	0	0	3.1**	0	0	0	0	0	0
	0.502 (77 %)													
	0.323 (47.2 %)													
CEM-IF	0.681 (84.7 %)	55.5	18.2	8.4	9.8	0	0	3.1**	0	0	0	0	0	0
	0.501 (78.7 %)													
	0.323 (59.1 %)													
CEM-H0	0.51 (82.4 %)	60.7	22.1	6.3	10.9	0	0	3.6	0	0	0	0	0	0
CEM-HQ	0.55 (91.3 %)	60.7	22.1	6.3	10.9	0	0	3.6	0	0	0	0	45	0
CEM-HS	0.53 (86.3 %)	60.7	22.1	6.3	10.9	0	0	3.6	0	0	45	0	0	0
CEM-HF	0.60 (85.6 %)	60.7	22.1	6.3	10.9	0	0	3.6	0	0	0	0	0	45
CEM-HL	0.54 (85.6 %)	60.7	22.1	6.3	10.9	0	0	3.6	0	45	0	0	0	0

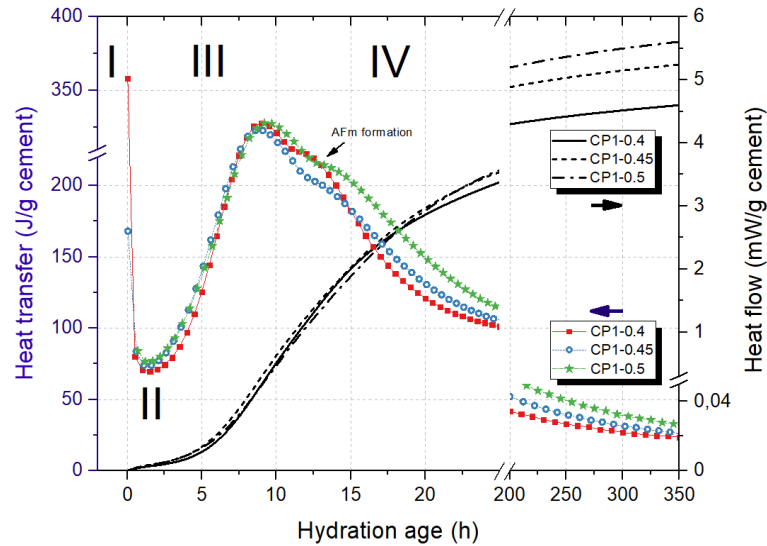
\* Contains both orthorhombic and cubic forms of C<sub>3</sub>A.

\*\* Data unavailable. The estimated values are derived from cements with similar composition.

† Includes all phases of added sulfates (gypsum or dihydrate, hemihydrate and anhydrite).

‡ w/b = water-to-binder ratio. doH = degree of hydration.

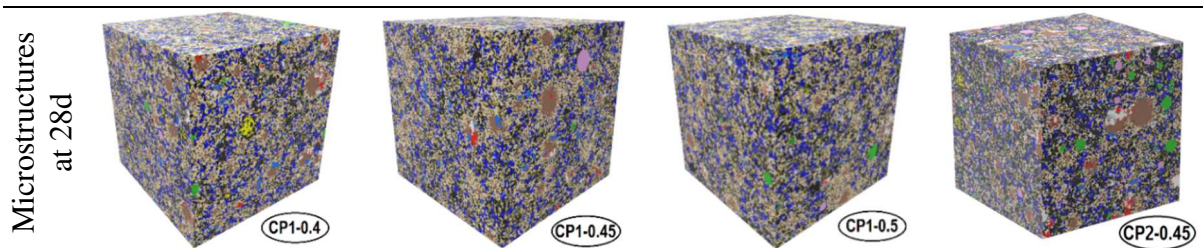
134 In order to relate each cycle with the correct hydration time and extract the microstructure at  
 135 28 days, isothermal calorimetry is conducted using the same cement paste compositions of the  
 136 first and second sets. In this experimental setup, the heat released by the hydration reactions is  
 137 recorded as a function of time, and then correlated to the heat release calculated by VCCTL,  
 138 as suggested by the hydration model's manual (Figure 1).  
 139



140  
 141  
 142  
 143

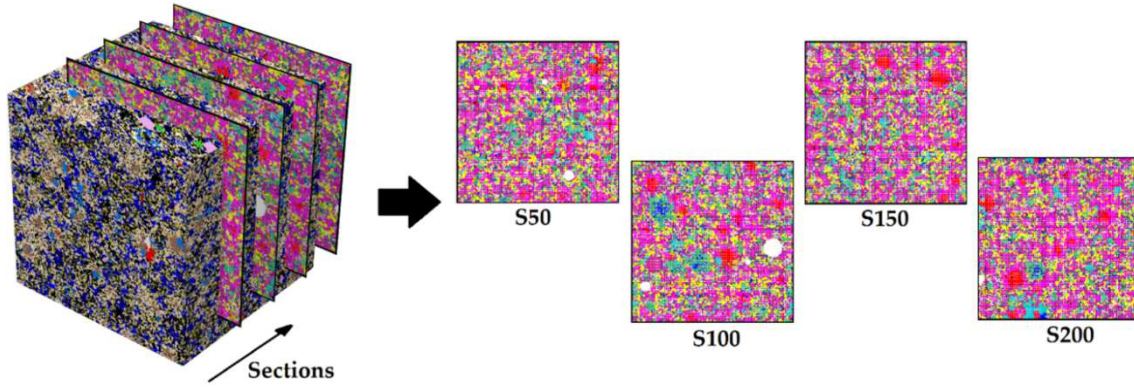
**Figure 1. Heat release during hydration of virtual cement pastes (from 0h to 24h, with a step of 5 hours, then up to 14 days).**

144 The virtual microstructure generated by VCCTL is shown in Figure 2. Since 3D simulations  
 145 were practically impossible due to the high number of voxels, 2D sections were extracted and  
 146 the simulations were conducted in 2D plane stress by considering a thin thickness. This  
 147 assumption is pertinent, because small displacements are considered, and, at each numerical  
 148 step, they are smaller than the thickness, far from the edge. The macroscopic results were  
 149 averaged over four sections (labelled S50, S100, S150 and S200, as illustrated in Figure 3). In  
 150 the finite element model, the different colours (or grey level) represent each cement paste's  
 151 components: *purple*=porosity, *red*= $C_3S$ , *orange*= $C_2S$ , *blue*= $C_3A$ , *light blue*= $C_4AF$ , *dark*  
 152 *blue*=sulfates, *white*=inert particles, *yellow*=CH, *pink*=C-S-H, *green*=hydrogarnet and AFm,  
 153 *light green*=ettringite (cf. 2D sections in Figure 3).  
 154



155

**Figure 2. 3D virtual cement pastes obtained by VCCTL.**



156

157

158

Figure 3. Extraction of sections S50, S100, S150 and S200 from the 3D microstructure.

## 159 2.2 Damage model

### 160 2.2.1 Problem formulation

161 Several models have been proposed for the simulation of damage in cementitious  
 162 materials. The model chosen to represent the local damage of cement phases inside the  
 163 microstructure is Fichant's model [31,35] based on the microplane model proposed in [36]  
 164 and the damage law of Mazars [37]. For the sake of simplicity, the isotropic description of the  
 165 model is used. According to the principles of damage theory, the effective stress tensor  $\tilde{\sigma}$  and  
 166 the total stress  $\sigma$  of the material can be expressed in terms of the elastic strain tensor such as:

$$\begin{aligned}\tilde{\sigma} &= \mathbb{C}^d \epsilon^e \\ \sigma &= \mathbb{C}^0 \epsilon^e\end{aligned}\quad (1)$$

167 where  $\mathbb{C}^d$  and  $\mathbb{C}^0$  denote the fourth-order stiffness tensors for damaged and undamaged states,  
 168 respectively. The relationship between the two tensors is given by [35]:

$$\mathbb{C}^d = (\mathbb{I} - \mathbb{D})\mathbb{C}^0 \quad (2)$$

169 where  $\mathbb{D}$  is the damage tensor, which can be simplified to  $\mathbb{D} = D\mathbb{I}$  in the isotropic case of the  
 170 model. In the absence of plasticity, the evolution of damage is controlled by the following  
 171 loading surface  $f$ :

$$f(\bar{n}) = \bar{n}\epsilon^e\bar{n} - \kappa_0 \quad (3)$$

172 To ensure that damage of cement phases grows only due to tension, only the tensile (positive)  
 173 components of the eigenstrain tensor are taken into account [37]. In this case, the equivalent  
 174 strain  $\epsilon_{EQ}$  is used:

$$\bar{n}\epsilon^e\bar{n} = \epsilon_{EQ} = \sqrt{\langle \epsilon_{11} \rangle_+^2 + \langle \epsilon_{22} \rangle_+^2 + \langle \epsilon_{33} \rangle_+^2} \quad (4)$$



175 where  $\epsilon_{ii}$  represents the eigenvalues of the strain tensor and  $\langle \cdot \rangle_+$  are the Macaulay brackets.  
 176 The evolution of the damage law due to tensile microcracking in the isotropic model takes the  
 177 following exponential form [38]:

$$\begin{cases} f = 0 \text{ and } \dot{\epsilon}_{EQ} > 0 \rightarrow \dot{D} = \frac{\kappa_0(1 + B_T \epsilon_{EQ})}{\epsilon_{EQ}^2} \exp[-B_T(\epsilon_{EQ} - \kappa_0)] \\ f < 0 \text{ or } \dot{\epsilon}_{EQ} = 0 \rightarrow \dot{D} = 0 \end{cases} \quad (5)$$

178 with  $\kappa_0$  denoting the strain damage threshold and  $B_T$  the strain softening slope parameter  
 179 which is linked to mode I fracture energy. These model parameters can be calculated from the  
 180 measurable mechanical properties of cement phases using the equations [38,39]:

$$\kappa_0 = \frac{f_t}{E} \quad B_T = \frac{f_t}{\frac{G_f}{h} - \frac{f_t \kappa_0}{2}} \quad (6)$$

181 where  $E$ ,  $f_t$  and  $G_f$  represent respectively the Young's modulus, tensile strength and fracture  
 182 energy of the cement phase. The above expression of  $B_T$  ensures that the energy dissipated in  
 183 a finite element during damage is independent of the mesh by introducing the characteristic  
 184 size  $h$  [38].

185 For the sake of simplicity, the same isotropic damage model was applied to all cement phases.  
 186 However, the mechanical parameters, namely  $E$ ,  $\nu$ ,  $f_t$  and  $G_f$ , differ from phase to phase (see  
 187 section 2.2.2). Damage in the cement paste is initiated by the local build-up of stress and  
 188 would progress through the weakest links in the material. It is assumed that the four  
 189 mechanical properties are not dependant on the cement paste mixture type and the test  
 190 conditions for each phase. It is rather the matrix's content and the phase assemblage that affect  
 191 the macroscopic behaviour of the cement paste.

## 192 **2.2.2 Elastic properties of the cement paste's phases**

193 Many researchers have measured elastic properties of the cement paste's components  
 194 (see references in the summary table 2). In this study, and for each elastic parameter, it is the  
 195 average of all the values found in the literature that is used in the simulations (Table 2). It  
 196 should be noted that these properties do not include the capillary porosity, which is modelled  
 197 as a separate "phase". The capillary porosity was given small values for the elastic properties  
 198 which were calibrated using experimental measurements of Young's modulus in cement paste  
 199 CP1-0.45 (following the suggested values in [40,41]). Elastic properties of C-S-H are  
 200 homogenized, assuming that C-S-H at the micro-scale is a mixture of 70% low density C-S-H  
 201 and 30% high density C-S-H [42].

**Table 2. Elastic properties of the cement paste phases.**

Cement phases		E (GPa)	$\nu$ (-)	Ref.	
Clinker phases	Alite	$C_3S$	137.4	0.299	[17,24,43–45]
	Belite	$C_2S$	135.5	0.297	[17,24,43–47]
	Celite	$C_3A$	145.2	0.278	[17,24,43–47]
	Ferrite	$C_4AF$	150.8	0.318	[17,24,43–46,48]
	Arcanite	$K\bar{S}$	44.2	0.269	[17,49]
	Thenardite	$N\bar{S}$	57.1	0.281	[17,48]
Gypsum	Gypsum	$C\bar{S}H_2$	44.5	0.33	[17,24,43,46,50]
	Bassanite	$C\bar{S}H_{0.5}$	132.0	0.25	[17,24,48]
	Anhydrite	$C\bar{S}$	88.8	0.233	[17,24,51]
Admixtures	Slags	$\S$	137.4	0.299	[17,24,43–45]
	Silica fume	$\S$	71.7	0.169	Same as $SiO_2$
	AS glass	$C_xS_yA_z$	71.7	0.169	Same as $SiO_2$
	Inert	$\S$	71.0	0.296	[21]
Main hydrates	Portlandite	$CH$	43.5	0.294	[17,24,32,43,52–54]
	C-S-H	$C_{1.7}SH_4$	23.8	0.24	[42,55]
	Hydro-garnet	$C_3AH_6$	93.8	0.32	[14,17]
	Ettringite	$C_6A\bar{S}_3H_{32}$	24.1	0.321	[14,17,24,32,43]
	Monosulfate	$C_4A\bar{S}H_{12}$	43.2	0.292	[14,17,24,32]
	Iron hydroxide	$FH_3$	22.4	0.25	[17]
	Calcite	$C\bar{C}$	97.0	0.296	[56]
Secondary hydrates	Limestone	$C$	183.9	0.21	[48]
	Iron-rich ettringite	$C_6(A.F)\bar{S}_3H_{32}$	24.1	0.321	Same as ettringite
	Pozzolanic / slag C-S-H	$\S$	23.8	0.24	Same as C-S-H
	Friedel's salt	$C_3A(CaCl_2)H_{10}$	22.4	0.25	[17]
	Strätlingite	$C_2ASH_8$	22.4	0.25	[17,57]
	Calcium mono-carbonate	$C_4A\bar{C}H_{11}$	79.0	0.25	[17,58]
	Brucite	$MH$	83.3	0.183	[57]
Magnesium sulphate	$M\bar{S}$	10.5	0.1	[59]	
Pores	Porosity (wet)	$H$	1.9	0.499	-
	Porosity (dry)	$\emptyset$	1.9	0.001	-

## 2.3 Numerical protocol for the determination of the damage properties of phases

The damage properties of the cement phases depend on their nature, morphology and porosity. For crystalline phases which exist naturally, or in the case of hydrates which can be synthesized, some mechanical properties have already been evaluated and can be founded in the literature (see [11,53,60] for a few examples). For other phases with a more complex nature such as C-S-H, nano-indentation or molecular dynamics simulations can be used. A review of the recent techniques that can be used to determine such properties is given in Zhang et al. [61].

It is important not to confound properties measured on pure materials with those of the porous phases in cement paste, as porosity considerably affects their mechanical properties. For instance, the Young's modulus of compacted ettringite powder is equal to 52 GPa while that of ettringite formed in cement paste is in the order of 25 GPa [17]. Since it is difficult to take into account all the heterogeneities of the cement paste, and due to the lack of damage properties of many phases, some assumptions are put forward for a numerical determination of these properties:

1. Each voxel in the finite element mesh corresponds to a unique homogenous phase,
2. All voxels of the same type have the same mechanical properties,
3. The behaviour of the phases is isotropic,
4. All phases obey the damage model presented above,
5. The tensile strength is proportional to the micro-hardness (or HD), according to a constant coefficient  $\alpha_{ft}$ , such as:  $HD = \alpha_{ft} \times f_t$ ,
6. The fracture energy of each phase is proportional to the elastic energy, according to a constant coefficient  $\beta_{Gf}$ , as follows:  $G_f = \beta_{Gf} \frac{(1+\nu)f_t^2}{E}$ .

Assumptions 1 and 3 decrease the number of elastic properties to two parameters:  $E$  and  $\nu$ . Assumptions 5 and 6 render it possible to write the relationship between unknown failure properties ( $f_t$  and  $G_f$ ) with other known properties which can be easily measured by nano-indentation ( $E$ ,  $\nu$  and  $HD$ ). For ductile materials, the empirical relation between hardness and strength is given by:  $HD = 3f_t$  [62]. For composites, granular materials, brittle glasses and ceramics, the proportionality coefficient is found between 28 and 200 [62].

The parameters  $\alpha_{ft}$  and  $\beta_{Gf}$  are assumed to be constants. This strong hypothesis is made considering that it is practically impossible to identify all the damage properties of the cement

235 phases. It is for this reason that the damage parameters found for the cement phases should be  
236 considered as “intrinsic” to the damage model being used here. However, unlike older studies  
237 [5,18] where the values given for the two parameters  $\alpha_{ft}$  and  $\beta_{Gf}$  are arbitrary, the parameters  
238 are fixed using an inverse analysis scheme. They are determined using the following strategy:

239 1. First, the mix design for the reference cement paste CP1-0.45 is prepared for  
240 experimental testing. Since cement paste is generally too brittle to effectively conduct  
241 direct tensile tests, CMOD-controlled three-point bending tests were conducted in  
242 sealed conditions to avoid drying-induced microcracking, as illustrated in Figure 4.  
243 The crack formation is monitored via the displacement called CMOD, or Crack Mouth  
244 Opening Displacement, which consists of the measurement of the lateral displacement  
245 of the notch at the bottom of the beam, representing the initial crack. The notch is  
246 carefully made by inserting a thin bar (~0.8mm) in the mould before casting the  
247 cement paste, as shown in Figure 4. Moreover, compressive strength was determined  
248 on 4x4x4cm cubic volumes of the same cement paste.

249



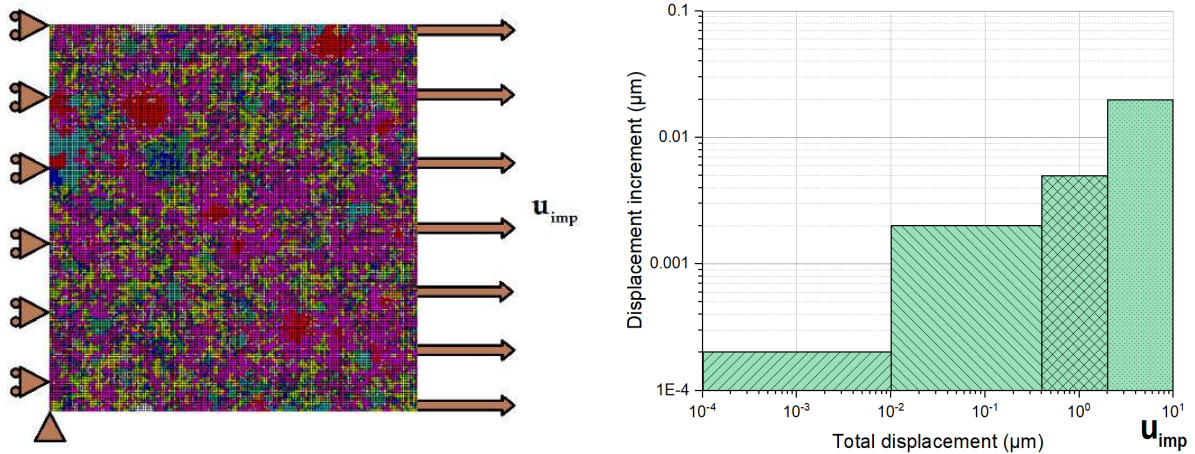
250 **Figure 4. Prepared cement paste beams for the CMOD-controlled three-point bending test.**

251

252 2. The unknown macroscopic properties of cement paste such as the tensile strength and  
253 the fracture energy were determined from the force-CMOD response obtained in the  
254 previous step using the methodology described in [63,64]. The obtained values for  
255  $f_{t,paste}$  and  $G_{f,paste}$  can then be used to determine  $\alpha_{ft}$  and  $\beta_{ft}$  in the following steps.

256 3. At the microscopic level, the virtual microstructure of CP1-0.45 is generated using  
257 VCCTL, as described above, and the REV is converted into a finite element mesh in  
258 the FE code Cast3M. The damage model is then applied to all phases, with the elastic  
259 properties given in Table 2 attributed to each corresponding phase. Initial values were  
260 given to  $\alpha_{ft}$  and  $\beta_{Gf}$  as a starting point for inverse identification. Isostatic boundary  
261 conditions have been applied with imposed displacement  $u_{imp}$  varying within the  
262 interval  $[0; 10\mu m]$ . The discretization of this interval is given in Figure 5. Indeed, the

263 displacement increment is not constant because the first steps require more precision  
 264 for computational convergence. This discretization is thus chosen as a compromise  
 265 between precision, convergence and speed. The final value of  $10\mu\text{m}$  is satisfactory  
 266 enough to obtain the total stress-crack opening curve, which allows for the calculation  
 267 of the numerical fracture energy from the softening slope.  
 268



269 **Figure 5. Numerical simulation of the tensile test: imposed boundary conditions (left) and imposed**  
 270 **displacement increments (right).**  
 271

- 272 4. The unknown parameters cannot be easily determined using optimization tools such as  
 273 the Levenberg-Marquardt method [65]. This is because both  $\alpha_{ft}$  and  $\beta_{Gf}$  influence the  
 274 macroscopic damage properties,  $f_t$  and  $G_f$ , in an unknown manner, and the solution  
 275 might not be unique. Therefore, an alternative is proposed, in the form of a design of  
 276 experiments (DOE). In this parametric study, numerical "experiments" are conducted  
 277 by simulating tensile and compressive tests on cement paste microstructures, which  
 278 can be used to determine their macroscopic properties. The influence of the parameters  
 279  $\alpha_{ft}$  and  $\beta_{Gf}$  can be established, and this allows for a quick determination of  $\alpha_{ft}$  and  $\beta_{Gf}$   
 280 without the need for the complicated algorithms of inverse analysis. This step is  
 281 explained in more detail in 3.1.
- 282 5. Once  $\alpha_{ft}$  and  $\beta_{Gf}$  are determined, the effective damage parameters of cement phases  
 283 are assumed to be independent of the cement paste mixture and test conditions, and  
 284 can be used in the damage model proposed above for other compositions. Only the  
 285 volume fractions and the distributions of the cement paste's phases inside the virtual  
 286 microstructure affect the global properties of the representative cement paste volume.  
 287

288

## 3 Results and discussion

289

### 3.1 Calculation of the damage properties of the cement paste's phases

290

Initial calculations showed that the adjustment of  $\alpha_{ft}$  and  $\beta_{Gf}$  affects simultaneously the tensile strength and the fracture energy of the cement paste CP1-0.45 at the macroscopic scale. If the micro-mechanical properties are to be determined, it must be proven that the inverse problem converges to a unique solution. This means that for a certain cement paste with given macroscopic properties, there is a unique couple  $(\alpha_{ft}, \beta_{Gf})$  which gives these properties.

295

296

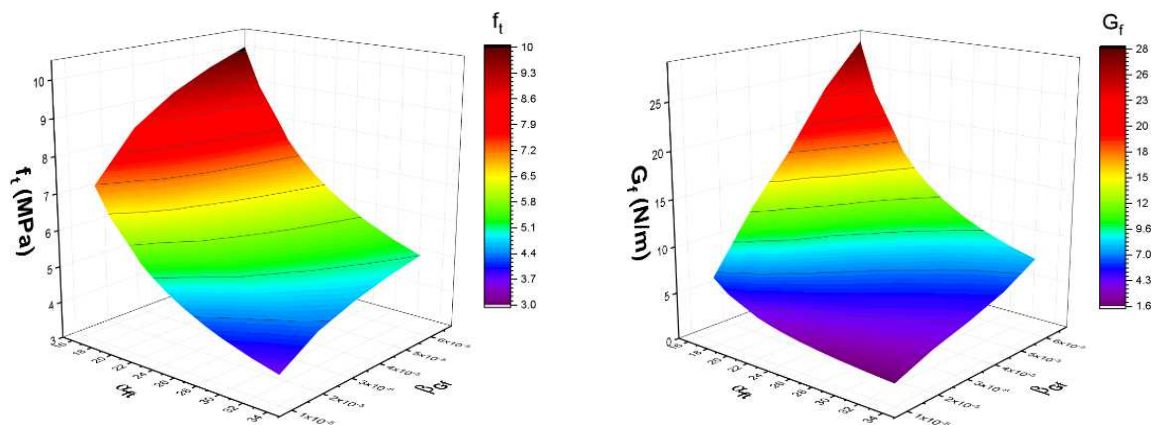
Let  $\mathcal{F}: \mathbb{R}^2 \rightarrow \mathbb{R}^2$  be defined as the function linking each couple of the micro-mechanical parameters  $(\alpha_{ft}, \beta_{Gf})$  to the macroscopic properties  $(f_t, G_f)$  of the cement paste. Tensile tests of the cement paste FC1-0.45 were simulated by varying  $\alpha_{ft}$  and  $\beta_{Gf}$  within the restricted domain  $[15; 35] \times [1.25 \times 10^{-5}; 6.25 \times 10^{-5}] \in \mathbb{R}^2$ . This domain is selected as it gives realistic values for  $f_t$  and  $G_f$ . The macroscopic properties, determined for each fixed value of  $(\alpha_{ft}, \beta_{Gf})$ , are mapped in Figure 6 as a function of two parameters. The results show that  $\mathcal{F}$  is subjective over the restricted domain of interest.

302

303

Therefore, the existence of the unique solution to the previous problem requires that  $\mathcal{F}$  be injective. In other words, the isocontours of  $f_t(\alpha_{ft}, \beta_{Gf})$  and  $G_f(\alpha_{ft}, \beta_{Gf})$  projected on the  $(\alpha_{ft}, \beta_{Gf})$  plane must always intersect at a unique point. The isocontours are lines that represent a constant value of the function  $\mathcal{F}$ .

306



307

308

Figure 6. Influence of  $\alpha_{ft}$  and  $\beta_{Gf}$  on the tensile strength (left) and on the failure energy (right).

309

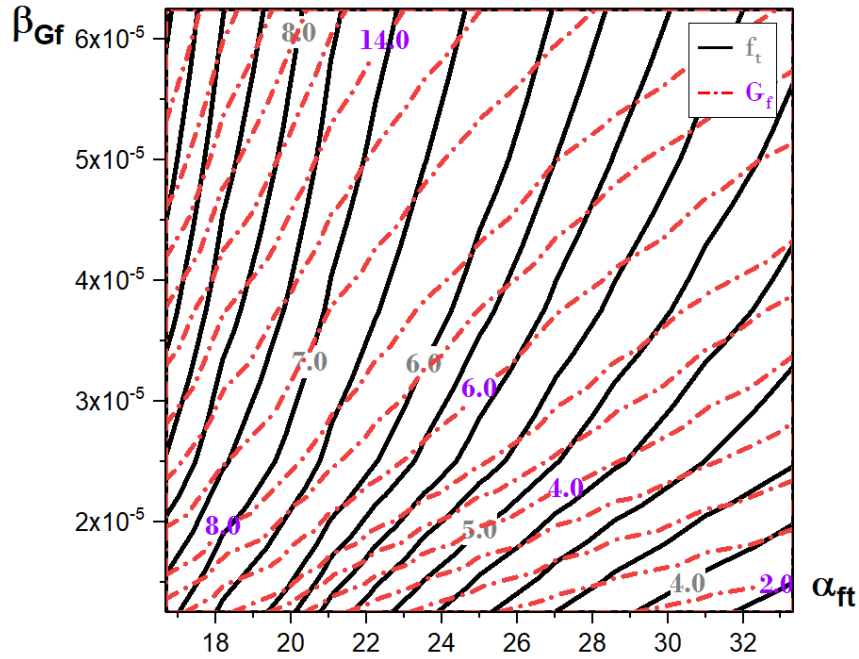
310 The projected isocontours of  $f_t$  and  $G_f$ , plotted in Figure 7, show that both  $\alpha_{ft}$  and  $\beta_{Gf}$  affect  
311 the strength and fracture energy of cement paste, with  $f_t$  strongly influenced by  $\alpha_{ft}$  and  
312 slightly increasing with  $\beta_{Gf}$  for low  $\alpha_{ft}$ . On the other hand,  $G_f$  is influenced equally by  $\alpha_{ft}$  and  
313  $\beta_{Gf}$ , but barely changes with respect to  $\alpha_{ft}$  when  $\beta_{Gf}$  is low.

314 This is expected, since any increase in the tensile strength of individual cement phases  
315 contributes to the total strength of the cement paste, while the increase of the fracture energy  
316 of phases with low tensile strength opposes the rapid development of damage and therefore  
317 slightly contributes to the overall strength. On the other hand, a low value for  $\beta_{Gf}$  means that  
318 cement paste's phases are very brittle, and the increase of their tensile strength will not  
319 contribute to the overall fracture energy. It can deduced from the pattern of the isocontours  
320 that, for any given value of  $(f_t, G_f)$ , there is a unique point of intersection in the restricted  
321 domain. This method makes it possible to directly determine the couple  $(\alpha_{ft}, \beta_{Gf})$  which  
322 coincides with the experimental values of  $f_t = 6.7$  MPa and  $G_f = 6.6$  J/m<sup>2</sup> corresponding to  
323 the reference cement paste CP1-0.45. The point of intersection, drawn in Figure 8, matches  
324 the determined values:  $\alpha_{ft} = 20.2$  and  $\beta_{Gf} = 3.75 \times 10^{-5}$ . This allows for calculating the  
325 damage properties of cement paste's phases, which are summarized in Table 3.

326 The obtained value for  $\alpha_{ft}$  suggests that the behaviour of cement paste's phases is, on average,  
327 more brittle than ductile metals ( $\alpha_{ft} = 3$ ), but remains less brittle than most ceramics ( $28 <$   
328  $\alpha_{ft} < 183$ ) [62]. The calculated tensile strength of C-S-H is equal to 55 MPa, which is lower  
329 than values of 264-700 MPa [53] or 66-107 MPa [32] found by other authors. On the other  
330 hand, the obtained fracture energy for C-S-H falls in the expected range of 4.4-20 J/m<sup>2</sup>  
331 [11,53]. This difference in the order of magnitude can be partially explained by the fact that  
332 the experimental values determined in [53] were flexural strengths measured on micro-beams  
333 which are not purely homogeneous, or due to the underlying assumptions made by the authors  
334 [32] regarding the hydrates.

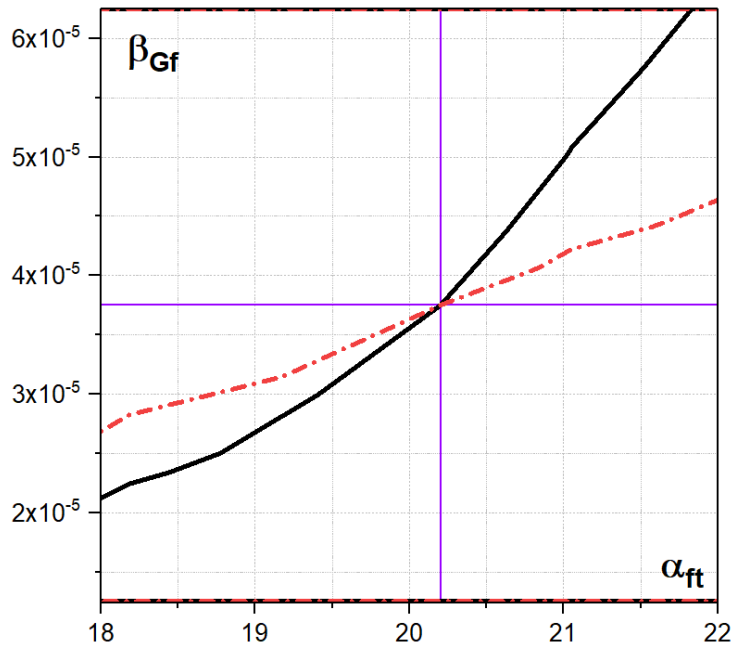
335 The assumptions taken here for the identification of the damage properties of cement paste's  
336 phases also affect the values found for the model parameters. It should therefore be  
337 understood that the properties found in this study are contingent on the damage model used  
338 for the behaviour of cement paste's phases. Nevertheless, these properties of cement paste's  
339 phase are not dependent on the composition of the microstructure.

340



341 **Figure 7.** Isocontours of the functions  $f_t$  (black solid lines) and  $G_f$  (red dashed lines) projected on  
 342 the  $(\alpha_{ft}, \beta_{Gf})$  plane. It is clear that: 1) the solid lines never cross each other, and the same goes for  
 343 the dashed lines, and 2) every red dashed line crosses any black solid line once and only once. The  
 344 two observations mean that, for any fixed values of  $f_t$  and  $G_f$ , the corresponding isocontours cross  
 345 at a unique point, which gives the unique values for  $(\alpha_{ft}, \beta_{Gf})$ .

346  
 347  
 348



349 **Figure 8.** Determination of the unique couple  $(\alpha_{ft}, \beta_{Gf})$  from the isocontours corresponding to the  
 350 experimental values of  $(f_t, G_f)$ .  
 351  
 352

353



**Table 3. Micro-mechanical damage properties of the main cement paste phases.**

Cement phases		$f_t$ (MPa)	$G_f$ (J/m <sup>2</sup> )	
Clinker phases	Alite	$C_3S$	430.7	65.8
	Belite	$C_2S$	396.0	56.3
	Celite	$C_3A$	534.6	94.3
	Ferrite	$C_4AF$	470.3	72.5
	Arcanite	$K\bar{S}$	29.7	1.0
	Thenardite	$N\bar{S}$	62.9	3.3
Gypsum	Gypsum	$C\bar{S}H_2$	29.6	1.0
	Bassanite	$C\bar{S}H_{0.5}$	61.7	1.4
	Anhydrite	$C\bar{S}$	93.6	4.6
Admixtures	Slags	§	430.7	65.8
	Silica fume	§	346.5	73.4
	AS glass	$C_xS_yA_z$	346.5	73.4
	Inert	§	69.3	3.3
Main hydrates	Portlandite	$CH$	73.8	6.1
	C-S-H	$C_{1.7}SH_4$	55.0	5.9
	Hydro-garnet	$C_3AH_6$	324.7	55.6
	Ettringite	$C_6A\bar{S}_3H_{32}$	39.6	3.2
	Monosulfate	$C_4A\bar{S}H_{12}$	262.4	77.3
	Iron hydroxide	$FH_3$	292.1	178.5
	Calcite	$C\bar{C}$	69.3	2.4
	Limestone	$C$	111.2	3.1
Secondary hydrates	Iron-rich ettringite	$C_6(A.F)\bar{S}_3H_{32}$	39.6	3.2
	Pozzolanic / slag C-S-H	§	55.0	5.9
	Friedel's salt	$C_3A(CaCl_2)H_{10}$	76.2	12.2
	Strätlingite	$C_2ASH_8$	328.2	225.4
	Calcium mono-carbonate	$C_4A\bar{C}H_{11}$	262.3	40.9
	Brucite	$MH$	49.5	1.3
	Magnesium sulphate	$M\bar{S}$	41.6	6.8
Pores	Porosity (wet)	$H$	0.001* 0.017**	~0* 0.02**
	Porosity (dry)	∅	0.001	~0

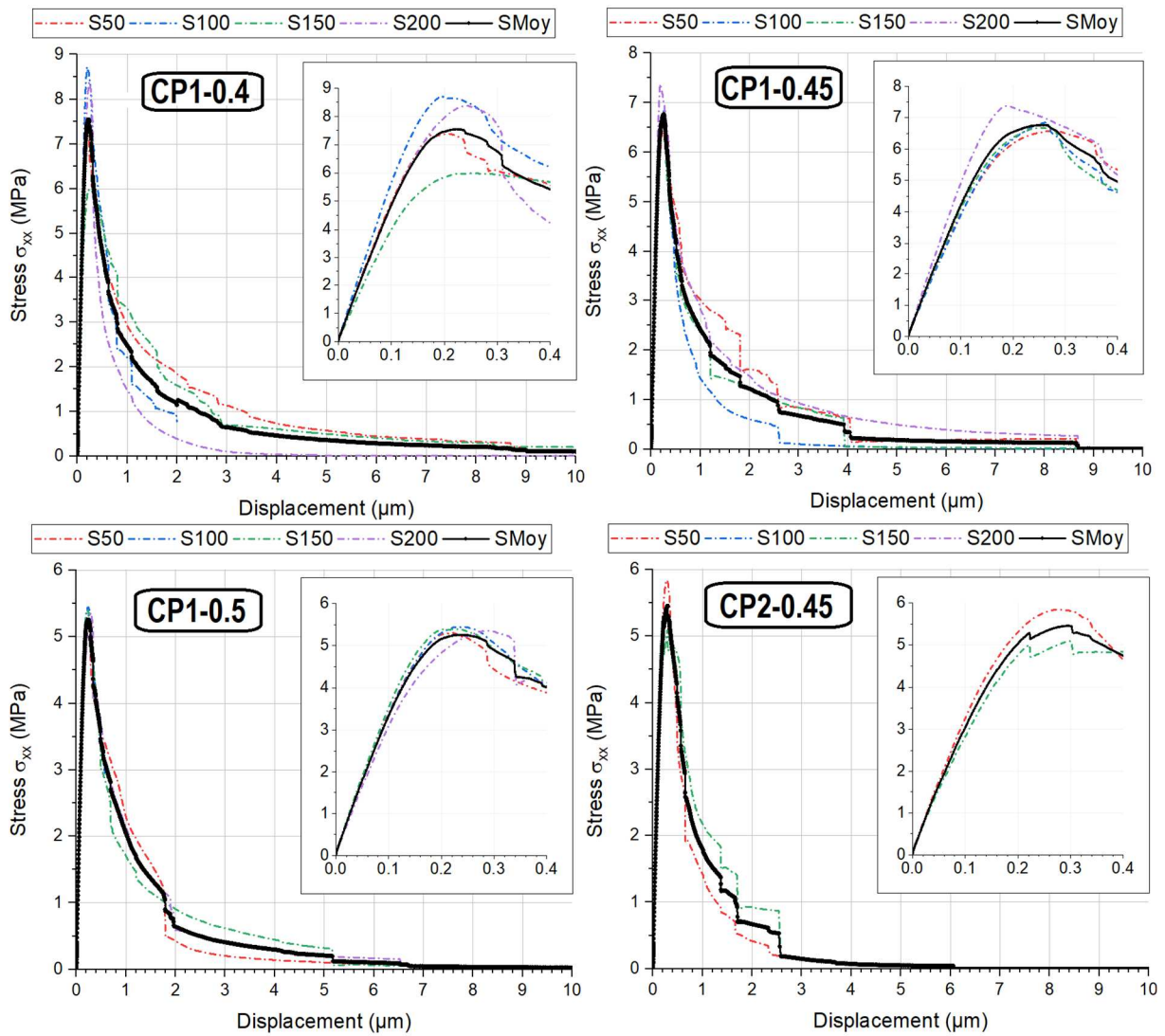
\* Calibrated for tension

\*\* Calibrated for compression

356 **3.2 Validation by a tensile failure test**

357 The macroscopic response along the direction  $i$  is calculated from the macroscopic  
 358 stress  $\Sigma_i$  and the strain  $E_i$ . However, in order to determine the macroscopic fracture energy,  
 359 the post-peak displacement due to crack opening,  $\Delta U_i^{pp}$ , is deduced from the computed  
 360 displacement field, as suggested in [39], and the macroscopic fracture energy is calculated as  
 361 the area below the  $\Sigma_i - \Delta U_i^{pp}$  curve.

362



363

364 **Figure 9. Macroscopic responses ( $\Sigma_X - \Delta U_X$ ) in tension for different cement paste compositions.**

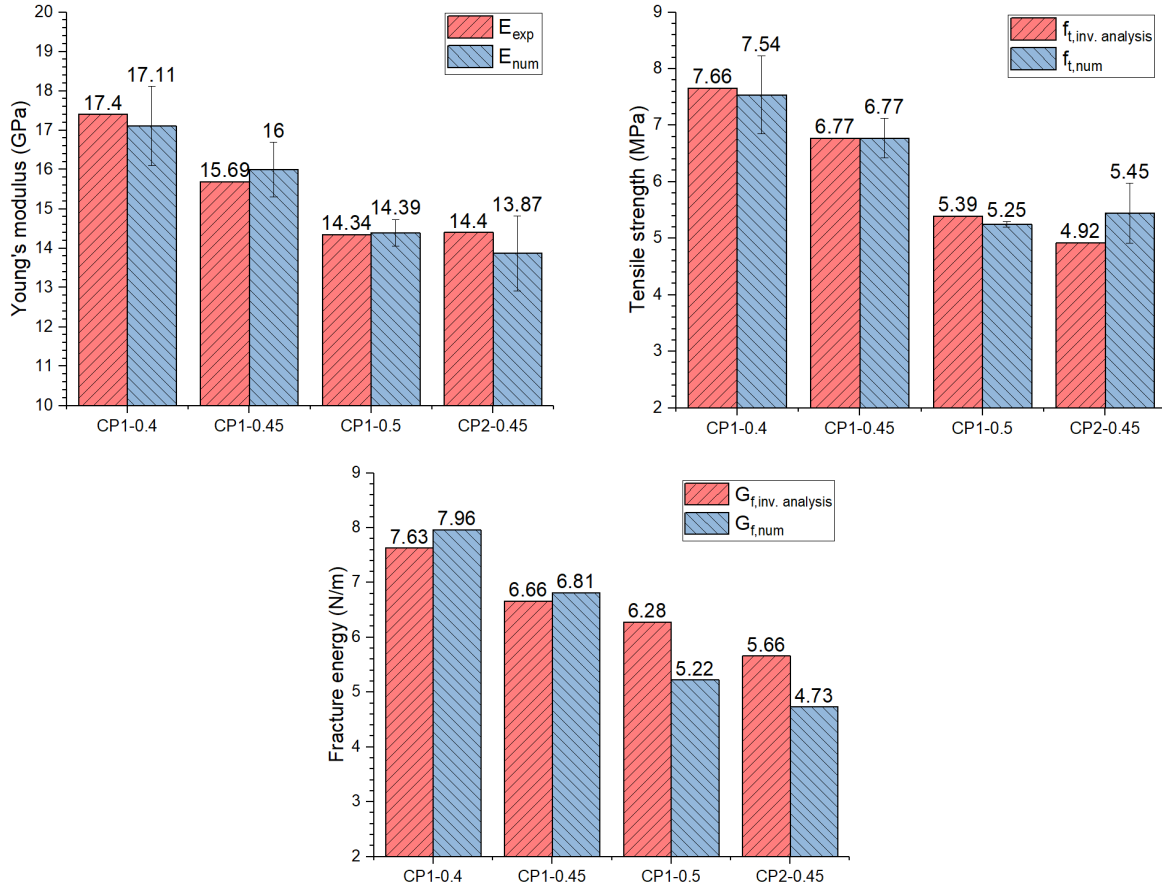
365

366 Figures 9 show the global stress-displacement response for CP1-0.45, as well as for the  
 367 second set of cement pastes FC1-0.4, CP1-0.5 and CP2-0.45, respectively. The inset graphs  
 368 represent the first stage of the response around the maximal stress values. The difference

369 between the behaviours along the two load directions  $X$  and  $Y$  amounts to less than 5%. For  
 370 this reason, only the responses along the  $X$  direction are shown.

371 The Young's modulus, the tensile strength and the fracture energy were calculated for the four  
 372 cement pastes and compared to experimentally-measured values, as shown in Figure 10.

373



374 **Figure 10. Comparison between numerical calculations and experimental measurements for  $E$ ,  $f_t$**   
 375 **and  $G_f$ .**

376

377 Error bars for the simulation results correspond to the differences between each simulated  
 378 sections of the cement paste volume. The Young's modulus  $E$  was determined from the initial  
 379 slope of the curve  $\Sigma_X - E_X$  in the pre-peak region, and no difference was found between the  
 380 two loading directions. The tensile strength  $f_t$  was identified as the maximal stress reached,  
 381 and  $G_f$  corresponds to the area under the  $\Sigma_X - \Delta U_X^{pp}$  curve.

382 Comparisons show that numerical results are in fairly good agreement with the experimental  
 383 values, even for the cement paste CP2 with a different cement containing calcite. This result  
 384 corroborates the proper selection of the REV and the model parameters for the phases. In  
 385 addition to that, the results show that the calibration made using only one cement paste to

386 determine the properties of the model is sufficient to simulate different cement paste  
387 compositions without the need for a new calibration of model parameters.

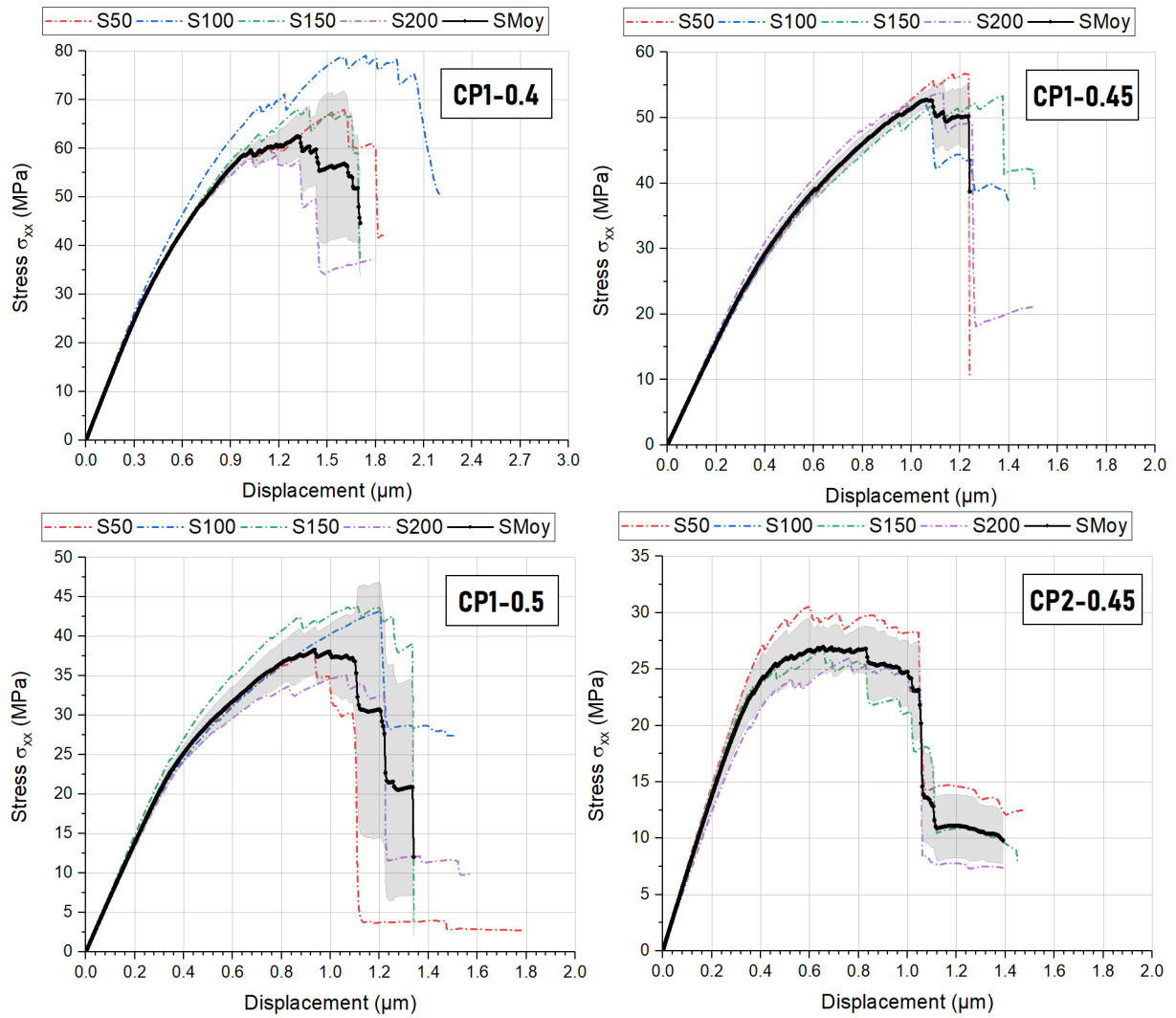
388

### 389 **3.3 Validation by a compressive test**

390 Using the above calculated parameters, compressive tests are simulated for all cement  
391 pastes and the results are compared to the experimental data. For the second set of cement  
392 pastes, the experimental compressive strength was determined using a classical compression  
393 test on  $4\times 4\times 4\text{cm}$  cubes. For the third set, cement paste microstructures were generated using  
394 VCCTL, based on the data available in the CemBase database [66]. Since the isothermal  
395 calorimetry curves of the cements were not given, hydration is simulated until the targeted  
396 degree of hydration which corresponds to the age at which the compression test is conducted  
397 by the authors of the CemBase, as shown in Table 1. The macroscopic stress-displacement  
398 curves of CP1-0.4, CP1-0.45, CP1-0.5 and CP2-0.45 are plotted in Figure 11: black lines  
399 (labelled SMoy) represent the average curve of the results obtained from the four sections,  
400 and the shaded areas represent the standard deviation.

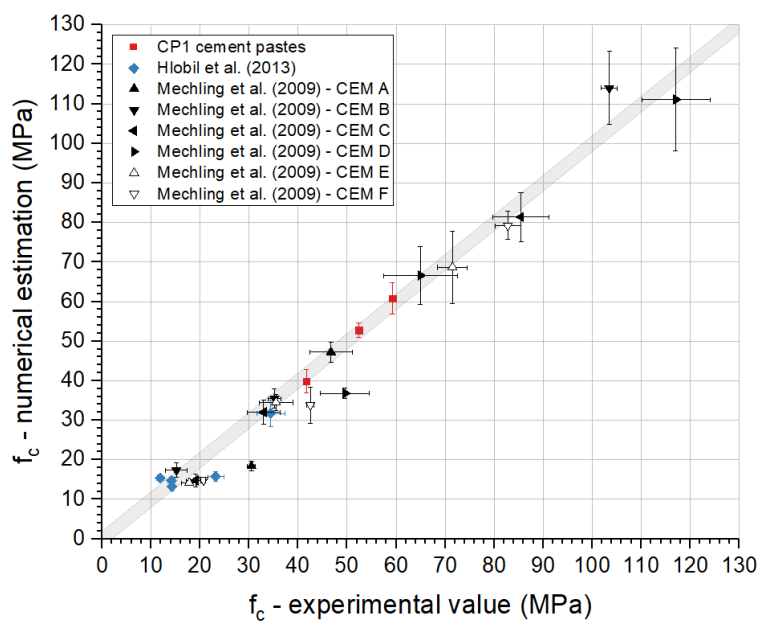
401 Calculations in compression were performed for more cement pastes containing mineral  
402 additions in place of cement. The numerical estimations for the compressive strength of all  
403 cement pastes are drawn against experimental values in Figure 12. This figure shows the  
404 relevance of the model to numerically estimate the compressive strength of low-carbon  
405 cement pastes. The shaded area corresponds to a margin of  $\pm 2$  MPa and the error bars  
406 represent the standard deviation.

407 Unlike in tension, the damage of cement paste in compression is not stable. For cement pastes  
408 made with CEM-N1, the applied stress drops sharply after reaching its peak value. For CP2-  
409 0.45 made from type II cement (CEM-N2), the stress maintains a steady state before total  
410 failure. This can be attributed to the presence of large pores left after the dissolution of  
411 calcium carbonate in CP2-0.45, which is mostly reactive due to its high amount in CEM-N2  
412 [67]. The presence of large pores acts as arrest mechanisms to the development of  
413 microcracks.



414  
415  
416

**Figure 11. Macroscopic responses in compression for different cement paste compositions.**



417  
418

**Figure 12. Compressive strengths of cement pastes: numerical-experimental comparison.**

419 As observed, the numerical value of the compressive strength for CP1 cement pastes matches  
420 the experimental results within a margin of  $\pm 2$  MPa (the experimental value for CP2-0.45 was  
421 not retrieved). For the third set of cement pastes, the lower the w/b ratio, the bigger the  
422 standard deviation between the numerical results of the same cement paste composition. This  
423 is also observed experimentally, and can be explained by the low porosity in compositions  
424 with low w/b ratios. For these compositions, the cement is only partially hydrated, and large  
425 particles of unhydrated clinker remain in the matrix. Therefore, these particles force the crack  
426 profile to change course between sections.

427 For the most part, the experimental results are predicted by the model to a satisfactory degree.  
428 In some cases, the modelling approach underestimates the compressive strength. This can be  
429 partially attributed to the lack of complete data regarding the cements from the CemBase  
430 database, such as the grading curve and the energy activation of cements, which were only  
431 assumed based on similar cements from the database of the hydration model. Nevertheless,  
432 the proposed model is able to provide quick estimations of the strength of cement pastes  
433 without adjusting any of its parameters.

434

### 435 **3.4 Use of the model for the analysis of the local damage at the micro-scale**

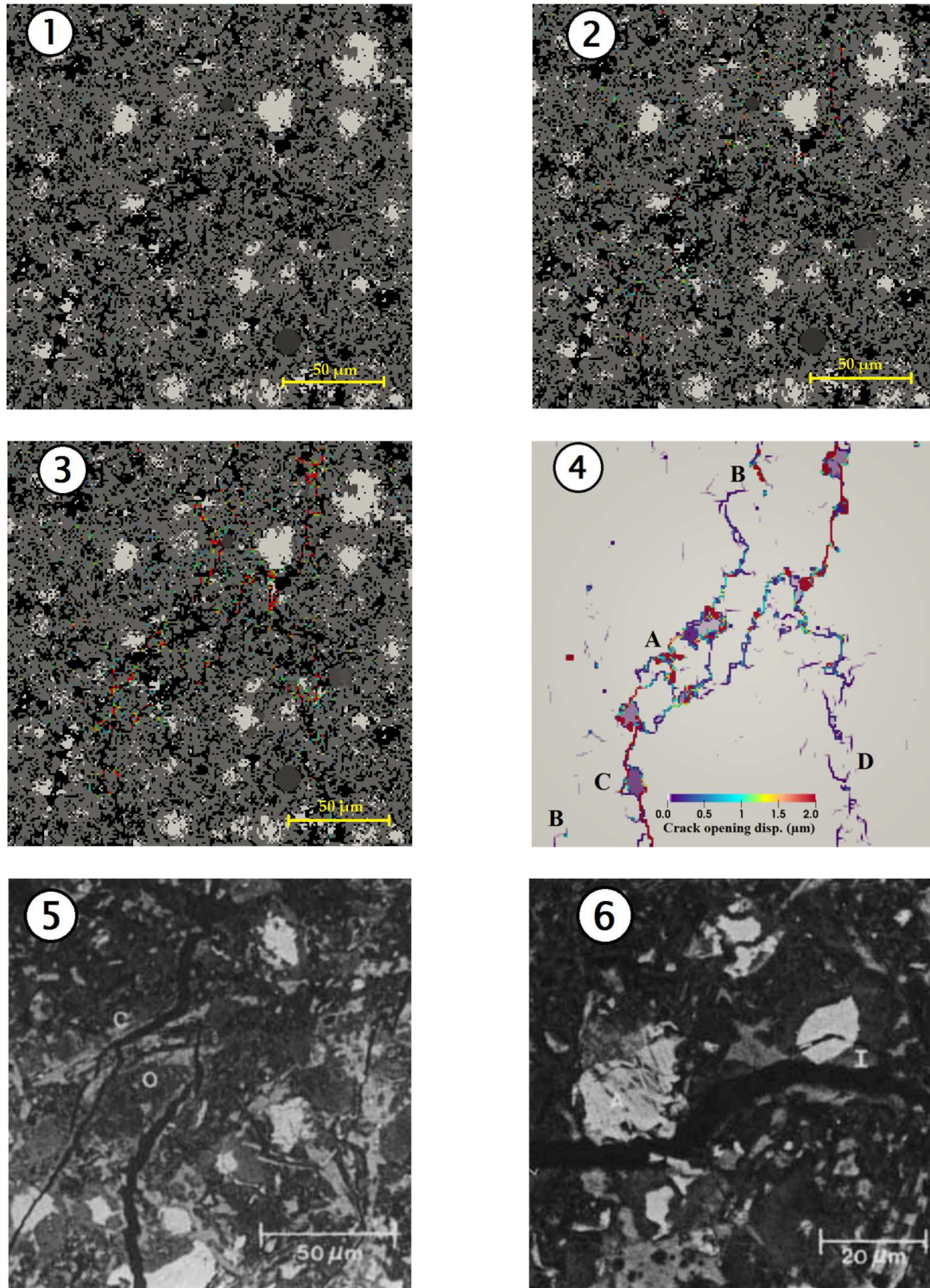
436 One important aspect of this micro-mechanical modelling approach is its ability to track  
437 the local behaviour which can be difficult to do during experimental testing. Using the model,  
438 it is possible to follow microscopic observations of mechanical shields during the test, the  
439 correlation between the cracking pattern and specific phases of the cement paste, the initiation  
440 and propagation of microcracks as well as the measurement of the crack openings, etc.

441 Figure 13 shows the damage maps extracted from CP1-0.45 at different steps of loading: at  
442 60% pre-peak, at the peak, and at 20% post-peak, with the crack opening profile at 20% post-  
443 peak calculated according to [39], and Scanning Electron Microscopic (SEM) observations of  
444 the crack pattern in cement pastes obtained from [68]. To clarify the illustration of cement  
445 phases, all anhydrous particles in the damage maps are shown in white, hydrates in grey and  
446 porosity in black.

447 It can be deduced that no significant damage occurs when 60% of the load is applied in the  
448 pre-peak region (only 18 finite elements are damaged). At the peak load, microcracks begin to  
449 coalesce and form short branches that develop mainly at the interface between anhydrous  
450 phases and hydrates, as shown in Figure 13-3 (numerical) and 13-6 (experimental). These  
451 branches remain for the most part unconnected, which provides cement paste with a softening

452 curve that is characteristic of a semi-stable fracture behaviour [8,69]. When the applied load  
453 reaches 20% in the post-peak region, microcracks merge to form major macrocracks that  
454 propagate along the weakest links and perpendicular to the loading direction. This is clearly  
455 observed in the crack opening profile in Figure 13-4.

456



457 **Figure 13.** Damage maps at 60% pre-peak (1), at the peak (2) and at 20% post-peak (3). Crack  
458 opening profile at 20% post-peak (4). Crack pattern obtained by SEM observations (5 and 6).  
459

460 When a crack reaches anhydrous particles, deviation and branching (A) occur due to the high  
461 resistance of clinker grains. This crack bifurcation is also observed in SEM images (cf. Figure  
462 12-5). In some cases, cracks can be arrested (B) or present offset (C) due to the presence of  
463 large portlandite crystals which remain undamaged. Microstructural features of crack also  
464 include the presence of a zigzag pattern (D) comprised of short segments  $\sim 10\mu\text{m}$  in length,  
465 which is attested by SEM observations by other authors [68].

466

## 467 **4 Conclusions and perspectives**

468 The presented study aims to contribute to the development of a numerical method for  
469 the determination of the damage properties of cement pastes for general use. In other words,  
470 the objective of this study is to provide a tool for rapid assessment of properties of different  
471 cement pastes, and therefore a tool that can be used for the optimization and the development  
472 of low-carbon concretes in order to decrease the climate impact of concrete industry.

473 For this reason, a micro-mechanical modelling approach is developed to identify the  
474 damage properties of all cement paste phases, including the mineral additions which are used  
475 in low-carbon cements. The method proposed to calculate these properties identifies values  
476 for the model parameters that are independent of the cement paste mixture and test conditions,  
477 and therefore can be used for any cement paste without calibration. Based on experimental  
478 data from nano-indentation tests found in the literature, the approach suggests calibrating only  
479 two parameters, which were remain constant for all cement paste compositions. This approach  
480 can be used in a similar way for other damage models, according to the number of unknown  
481 parameters. Simulations of both tensile and compressive tests are conducted on cement pastes  
482 with various mix designs, including low-carbon cement pastes, and then compared to the  
483 measured experimental values. The results demonstrate the utility of the modelling approach  
484 to estimate the properties of cement pastes, including strengths and fracture energy, without  
485 resorting to experimental tests or repetitive fitting of model parameters.

486 Because the model gives the global mechanical response of the cement paste, it is then  
487 possible to extract the homogenized properties and use them at the upper scale (i.e. mortar and  
488 concrete scales). This provides a calibration-free method to quickly assess the main properties  
489 of different concrete in order to optimize their mix designs. The approach also allows for a  
490 close investigation of microcracking patterns and crack profiles. First tests were conducted at  
491 the mortar scale for an ordinary cement to simulate the failure of mortar beams [70]. On



492 another note, coupling the mechanical damage with thermal, hydraulic or chemical processes  
493 and phenomena is possible, starting at the microscale. This allows for a better evaluation of  
494 the damage patterns that involve complex multi-physics simulations. Evaluations of the sort,  
495 such as freeze-thaw cycles, high temperatures, creep and shrinkage, have been performed and  
496 analysed in order to validate the models, and will be published following the basics of the  
497 proposed approach. A decision-making tool for concrete suppliers can therefore be utilized for  
498 optimization and evaluation of material properties and behaviours.

499

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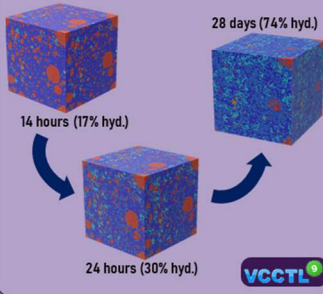
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# Micro-mechanical model

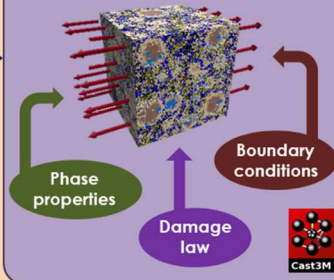
## Hydration simulation

The gradual hydration of the cement paste is processed via a hydration model, giving a representative virtual microstructure of the real cement paste.



## Finite-element modelling

The intrinsic behaviour of the phases in the cement paste is reproduced using a damage model with phase properties that are known. Different boundary conditions can be imposed



### What the model needs:

- Mineral composition of cement.
- Particle size distribution of cement.
- Water-to-binder ratio.
- Activation energy of cement.
- Temperature.
- Mass fractions of mineral additives, if any.
- No tedious experiment is needed.

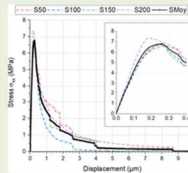


Cement paste with unknown properties

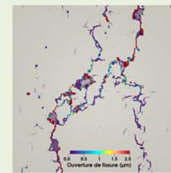
### What the model provides:

$E$	$\nu$	$f_t$	$G_f$
15GPa	0,24	6MPa	8J/m <sup>2</sup>

Mechanical properties of cement paste (needed for upscale modelling of concrete)



Mechanical behaviour



Cracking patterns



Mechanical behaviour determined!