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Discrete modeling of concrete failure and size-effect

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Abstract

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Size-effect in concrete and other quasi-brittle materials defines the relation between the nominal strength and structural size when material fractures. The main cause of size-effect is the so-called energetic size-effect which results from the release of the stored energy in the structure into the fracture front. In quasi-brittle materials and in contrast to brittle materials, the size of the fracture process zone is non-negligible compared to the structural size. As a consequence, the resulting size-effect law is non-linear and deviates from the response predicted by linear elastic fracture mechanics. In order to simulate the size-effect, one needs to rely on numerical modeling to describe the formation, development and propagation of the fracture process zone. Although a number of models have been proposed over the years, it transpires that a correct description of the fracture and size-effect which accounts for boundary effects and varying structural geometry remains challenging. In this study, the Lattice Discrete Particle Model (LDPM) is proposed to investigate the effects of structural dimension and geometry on the nominal strength and fracturing process in concrete. LDPM simulates concrete at the aggregate level and has shown superior capabilities

in simulating complex cracking mechanisms thanks to the inherent discrete nature of the model. In order to evaluate concrete size-effect and provide a solid validation of LDPM, one of the most complete experimental data set available in the literature was considered and includes three-point bending tests on notched and unnotched beams. The model parameters were first calibrated on a single size notched beam under three-point bending and on the mechanical response under unconfined compression. LDPM was then used to perform blind predictions on the load-crack mouth opening displacement curves of different beam sizes and notch lengths. Splitting test results on cylinders were also predicted. The results show a very good agreement with the experimental data. The quality of the predictions was quantitatively assessed. In addition, a discussion on the fracturing process and dissipated energy is provided. Last but not least, the Universal Size-Effect Law proposed by Bažant and coworkers was used to estimate concrete fracture parameters based on experimental and numerical data.

Keywords: Concrete failure, Size-effect, Effect of geometry, Lattice Discrete Particle Model, Numerical modeling, Energy dissipation

1. Introduction

Size-effect in quasi-brittle materials has been extensively investigated in the literature experimentally, theoretically, and numerically. In these materials, a reduction in strength is observed when the structural size increases in geometrically similar structures. This phenomenon has been confirmed for concrete (see for instance the work of Bažant and Pfeiffer (1987); Hoover et al. (2013); Grégoire et al. (2013); Çağlar and Şener (2016)) and its importance was acknowledged in the civil engineering community, as it was for the first time incorporated in the most recent ACI standard in 2019 (ACI-Committee, 2019). Two main reasons explain this size-effect (Bažant and Planas, 1997; Bažant, 2002; Bažant and Le,

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2017). The first one is the redistribution of stress due to stable crack propagation and re-
lease of stored energy into the fracture front. The second reason is the spatial randomness
in material properties. In this study, only size-effect due to stress redistribution is studied,
i.e. the energetic size-effect which is, in passing, purely deterministic. In concrete, the size
of the fracture process zone (FPZ) is non-negligible as compared to the structural size and
a complete non-linear theoretical fracture mechanics framework does not exist. Simplified
analytical formulations such as Bažant’s size-effect law (Bažant, 2002) only provide an ap-
proximate description of concrete scaling law. In order to account for the release of the
stored energy in the FPZ, and for the development and propagation of the fracture front
for different specimen sizes and shapes, one must carry out accurate numerical simulations.
Several types of models have been proposed over the years to describe concrete fracture
and size-effect. One can mention for instance the cohesive model (Elices et al., 2002), the
crack-band model (Bažant and Oh, 1983), non-local continuum damage models (Bažant
and Jirásek, 2002), and discrete models (Bolander et al., 2021). In all the aforementioned
formulations, two features are essential in capturing size-effect in strain softening materials
such as concrete: (i) crack localization and (ii) existence of an internal characteristic length
related to the size of the heterogeneity. In continuum models, these two ingredients are
phenomenologically defined through constitutive laws. In this respect, random lattice or
particle models such as the ones described by Cusatis et al. (2011a) or Eliáš et al. (2015)
are considered superior. The actual mix design and particle size distribution can be simu-
lated to produce a realistic heterogeneous internal structure made of interacting aggregates.
In addition, the randomness in spatial distribution of particles reproduces the statistically
isotropic nature of concrete and eliminates directional mesh bias during the fracturing pro-
cess. Finally, a recent argument in favor of lattice particle models is their ability to capture
the effect of stress parallel to cracks on the FPZ size and the induced size-effect, which was
demonstrated to be significant in concrete (Nguyen et al., 2020a,b). In this study, one of
such models, namely the Lattice Discrete Particle Model (LDPM) (Cusatis et al., 2011a,b)
which simulates concrete at the coarse aggregate level is adopted.

In order to assess the capabilities of LDPM in simulating fracture and predicting size-

39 effect, a comprehensive experimental data set on concrete fracturing (Grégoire et al., 2013)
40 was considered in this study. This data set is among one of the very few available in the
41 literature that includes three-point bending tests on notched and unnotched beams and
42 encompasses a large range of beam depths. It should be mentioned that this set of data
43 was previously used in several studies involving other numerical models. More specifically,
44 an integral-type non-local model was used but was found ineffective in capturing correct
45 size and geometry effects (Grégoire et al., 2013). In another study, a lattice model (Grassl
46 et al., 2012) was able to simulate the data with a good accuracy. It must however be
47 noted that the latter model falls into the miniscale category which implies computationally
48 prohibitive simulations for more complex geometries that require an increase in structural
49 size or account for the third dimension in the out-of-plane direction. It should also be
50 mentioned that the model used in that study was bidimensional and that to the authors
51 knowledge, there has been no attempt to extend the simulations to the 3D case. More
52 recently, a study proposed to simulate concrete fracturing using a local isotropic damage
53 constitutive model of the Rankine type through the crack band model (Barbat et al., 2020).
54 Although a good agreement with experimental data was found, this type of smeared crack
55 model is limited in capturing complex cracking mechanisms and realistic crack tortuosity
56 observed in concrete, which might have a non-negligible effect on energy dissipation during
57 fracture. As a matter of fact, this effect is especially important in the case of unnotched
58 beams where a large damage zone is generated before its collapse to a single propagating
59 crack that is ultimately tortuous and not straight. Last but not least, a re-implementation of
60 LDPM which includes stochasticity in material parameters was recently used to simulate the
61 data used in this paper (Eliáš and Vořechovský, 2020) with a very good accuracy. It should
62 be however emphasized that the latter study did not assess the capability of the model to
63 predict size-effect. Indeed, the study used all the load-crack mouth opening displacement
64 (CMOD) curves for all the beam sizes and notch lengths in the calibration process, with the
65 exception of the unnotched beams and the smallest sizes that were discarded.

66 In this work, the relevant LDPM parameters were calibrated on a single beam configura-
67 tion, leaving the remaining fracture test results for blind predictions, including splitting

68 tests. In addition and in contrast with most available studies, a rigorous quantification of
69 the prediction accuracy was performed. It is the wish of the authors that this work would,
70 to some extent, pave the way for more detailed and quantitative analyses of goodness of fits
71 and prediction quality in future numerical studies within the concrete community, using the
72 same set of experimental data but possibly other data. This would ultimately allow one to
73 compare different model capabilities, develop the most effective models and abandon the less
74 accurate ones. The proposed approach and preliminary results were presented in a recent
75 conference (Pathirage et al., 2022b,a; Pijaudier-Cabot et al., 2022). They are here largely
76 extended and commented.

77 **2. The Lattice Discrete Particle Model**

78 In order to simulate the FPZ formation and propagation in concrete necessary to cap-
79 ture size-effect, the Lattice Discrete Particle Model is here adopted. This model originally
80 proposed by Cusatis and coworkers (Cusatis et al., 2011a,b) simulates the mechanical inter-
81 actions among major material heterogeneities, i.e. coarse aggregates in concrete. Over the
82 years, this model has been used to simulate other granular quasi-brittle materials such as
83 mortar (Pathirage et al., 2019b; Han et al., 2020), fiber reinforced concrete and engineered
84 cementitious composites (Schauffert and Cusatis, 2011; Rezakhani et al., 2021; Feng et al.,
85 2022), unreinforced and reinforced stone masonry (Mercuri et al., 2020; Angiolilli et al.,
86 2020, 2021; Mercuri et al., 2022, 2021), shale (Li et al., 2017), or cycling in concrete (Zhu
87 et al., 2022). LDPM was also coupled to multi-physics models describing cement hydra-
88 tion from microscale simulations, heat transfer and moisture diffusion, alkali-silica reaction,
89 creep, aging (Alnaggar et al., 2013; Pathirage et al., 2019a; Yang et al., 2021, 2022), or more
90 recently self-healing in concrete (Cibelli et al., 2022).

91 *2.1. Internal geometry*

92 In order to generate the LDPM skeleton, spherical particles are placed in a volume of
93 material from the largest to smallest size. This placement follows a prescribed particle size
94 distribution that is based on the actual concrete mix design with the maximum and minimum

95 aggregate sizes, d_a and d_0 , respectively. Figure 1(a) shows an example of particle placement
 96 in a prismatic sample. In order to simulate the interaction between particles, a lattice system
 97 is generated by means of a Delaunay tetrahedralization with the centers of particles. A dual
 98 tessellation is then performed which finally produces a system of polyhedral cells enclosing
 99 the spherical particles. Figure 1(b) shows an example of two adjacent polyhedral cells
 100 enclosing the spherical particles. One can also refer to Figures 22(b)-(d) where cells at the
 101 surface of prismatic samples are depicted. The surface of each polyhedral cell is composed of
 102 triangular facets where failure can potentially occur. On each facet, stresses and strains are
 103 formulated in a vectorial form through constitutive equations. Figure 1(c) shows the three
 104 unit vectors defined at a generic facet colored in red, in the normal direction and in the two
 105 tangential directions. LDPM incorporates specific constitutive equations to describe tensile
 106 fracturing with strain softening, cohesive and frictional shearing, and compressive response
 107 with strain-hardening. Since this study focuses on concrete fracturing, the corresponding
 108 constitutive laws are detailed in the following. The reader is referred to the Appendix for
 109 the complete set of constitutive equations.

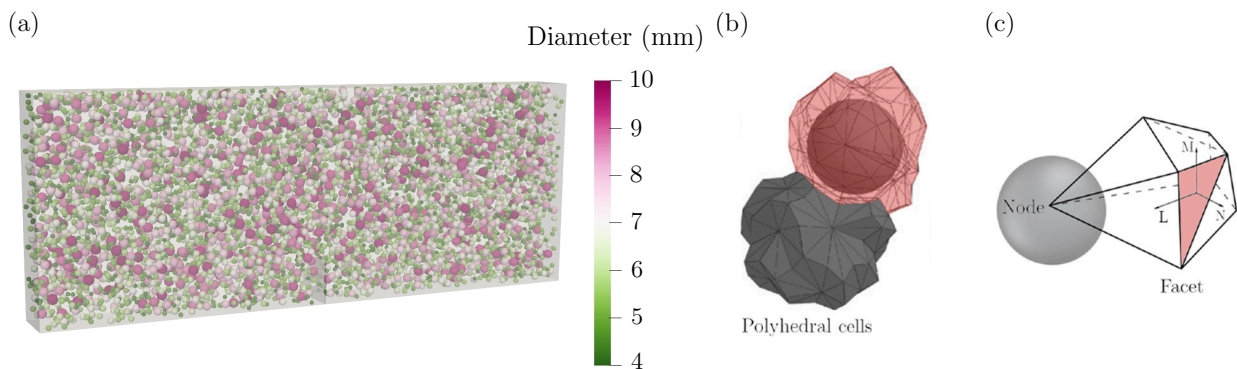


Figure 1: LDPM internal geometry: (a) particle placement in a prismatic volume, (b) two adjacent LDPM cells, and (c) triangular facet and vector orientations.

110 *2.2. Elastic, tension, and tension-shear constitutive behaviors*

111 If \mathbf{x}_i and \mathbf{x}_j denote the positions of nodes i and j , adjacent to the facet k , the facet
112 strains are defined as:

$$\mathbf{e}_k = [e_{N_k} \ e_{M_k} \ e_{L_k}]^t = \left[\frac{\mathbf{n}_k^t \llbracket \mathbf{u}_k \rrbracket}{l_k} \ \frac{\mathbf{m}_k^t \llbracket \mathbf{u}_k \rrbracket}{l_k} \ \frac{\mathbf{l}_k^t \llbracket \mathbf{u}_k \rrbracket}{l_k} \right]^t \quad (1)$$

113 where e_{N_k} is the normal strain component, and e_{M_k} and e_{L_k} are the tangential strain com-
114 ponents, $\llbracket \mathbf{u}_k \rrbracket = \mathbf{u}_j - \mathbf{u}_i$ is the displacement jump corresponding to facet k , $l_k = \|\mathbf{x}_j - \mathbf{x}_i\|$ is
115 the distance between the two nodes, $\mathbf{n}_k = (\mathbf{x}_j - \mathbf{x}_i)/l_k$ and \mathbf{m}_k and \mathbf{l}_k are two unit vectors
116 mutually orthogonal in the facet plane projected orthogonally to the line connecting the
117 adjacent nodes. The traction vector is defined as $\mathbf{t}_k = [t_{N_k} \ t_{M_k} \ t_{L_k}]^t$, where t_{N_k} is the normal
118 component, and t_{M_k} and t_{L_k} are the shear components. For the sake of readability, the
119 subscript k that designates the facet is dropped. The elastic behavior is formulated through
120 linear relations between the normal and shear stresses, and the corresponding strains as
121 follows:

$$t_N = E_N e_N, \quad t_M = E_T e_M, \quad t_L = E_T e_L \quad (2)$$

122 where $E_N = E_0$ and $E_T = \alpha_0 E_0$. $E_0 \approx E/(1 - 2\nu)$ and $\alpha_0 \approx (1 - 4\nu)/(1 + \nu)$ are the
123 effective normal modulus and the shear-normal coupling parameter, respectively, and E is
124 the macroscopic Young's modulus and ν is the macroscopic Poisson's ratio.

125 Because of the mesoscale nature of the model, concrete fracturing in mode I opening is
126 always accompanied by shear at facets. This is a realistic feature since it is experimentally
127 observed that most fracture paths are located at the interface between aggregates and cement
128 paste. Therefore, the cohesive fracture behaviors in tension but also in tension-shear are
129 important. This cohesive fracture occurs for $e_N > 0$. One can define an effective strain
130 as $e = (e_N^2 + \alpha_0(e_M^2 + e_L^2))^{\frac{1}{2}}$, and an effective stress as $t = (t_N^2 + (t_M^2 + t_L^2)/\alpha_0)^{\frac{1}{2}}$ and
131 write the relationship between stresses and strains through $t_N = te_N/e$, $t_M = \alpha_0 te_M/e$ and
132 $t_L = \alpha_0 te_L/e$. The effective stress t is defined incrementally as $\dot{t} = E_N \dot{e}$ and its magnitude
133 is limited by a strain-dependent boundary which is written as $0 \leq t \leq \sigma_{bt}(e, \omega_{sn})$ where

$$\sigma_{bt}(e, \omega_{sn}) = \sigma_0(\omega_{sn}) \exp \left[-H_0(\omega_{sn}) \frac{\langle e_{\max} - e_0(\omega_{sn}) \rangle}{\sigma_0(\omega_{sn})} \right] \quad (3)$$

134 $\langle x \rangle = \max(x, 0)$, ω_{sn} is a variable defining the level of interaction between shear and normal
 135 loadings. It is defined as $\tan(\omega_{sn}) = (e_N)/(\sqrt{\alpha_0}e_T) = (t_N\sqrt{\alpha_0})/(t_T)$ where e_T is the total
 136 shear strain $e_T = (e_M^2 + e_L^2)^{\frac{1}{2}}$, and t_T is the total shear stress $t_T = (t_M^2 + t_L^2)^{\frac{1}{2}}$. The maximum
 137 effective strain is time dependent and is defined as $e_{\max}(\tau) = (e_{N,\max}^2(\tau) + \alpha_0 e_{T,\max}^2(\tau))^{\frac{1}{2}}$
 138 where $e_{N,\max}(\tau) = \max_{\tau' < \tau}[e_N(\tau')]$ and $e_{T,\max}(\tau) = \max_{\tau' < \tau}[e_T(\tau')]$. The strength limit of the
 139 effective stress that defines the transition between pure tension and pure shear is written as

$$\sigma_0(\omega_{sn}) = \sigma_t \frac{-\sin(\omega_{sn}) + (\sin^2(\omega_{sn}) + 4\alpha_0 \cos^2(\omega_{sn})/r_{st}^2)^{\frac{1}{2}}}{2\alpha_0 \cos^2(\omega_{sn})/r_{st}^2} \quad (4)$$

140 where $r_{st} = \sigma_s/\sigma_t$ is the ratio of the shear strength to the tensile strength, σ_s is the shear
 141 strength and σ_t is the tensile strength. The post-peak softening modulus is controlled
 142 by the effective softening modulus $H_0(\omega_{sn}) = H_s/\alpha_0 + (H_t - H_s/\alpha_0)(2\omega_{sn}/\pi)^{n_t}$, in which
 143 $H_t = 2E_0/(l_t/l - 1)$, $H_s = r_s E_0$ and n_t is the softening exponent. Typically, the values of
 144 $n_t = 0.2$ and $r_s = 0$ are assumed and are fixed. l_t is the tensile characteristic length defined
 145 as $l_t = 2E_0 G_t/\sigma_t^2$ and G_t is the mesoscale fracture energy.

146 2.3. Static equilibrium equations and numerical implementation

147 Finally, one can write the static linear and angular momentum equilibrium equations of
 148 each LDPM cell as follows:

$$\sum_{k \in \mathcal{F}_I} A_k^p \mathbf{t}_k = \mathbf{0}, \quad \sum_{k \in \mathcal{F}_I} A_k^p \mathbf{c}_k \times \mathbf{t}_k = \mathbf{0} \quad (5)$$

149 where \mathcal{F}_I is the set containing all the facets of a generic polyhedral cell I , $A_k^p = A_k \mathbf{n}^t \mathbf{n}_k$ is
 150 the area of the projected facet k , \mathbf{n} is the orientation of the tetrahedron edge associated to
 151 facet k and \mathbf{n}_k is the unit vector orthogonal to facet k of area A_k (Cusatis et al., 2011a). \mathbf{c}_k
 152 is the vector that represents the distance between the center of facet k and the center of the
 153 cell. The model was implemented within a dynamic explicit scheme, with a central difference
 154 algorithm for time integration. Although the actual equations that are solved numerically
 155 are dynamic (see Cusatis et al. (2011a) for more details), the inertia terms are absent in the
 156 two expressions in Equation 5 because all the simulations presented next were performed
 157 under quasi-static conditions. In other words, loading rates were small enough to ensure

158 the kinetic energy in the system would not exceed 5% of the internal energy throughout the
159 analysis.

160 3. Regression statistics

161 Before describing the modeling and calibration process, it is important to introduce the
162 regression statistics used in this work to perform the model parameter identification and
163 list the different statistical indicators used to assess the quality of fit and the quality of
164 predictions. In this study, a frequentist approach is proposed.

165 3.1. Experimental data and model response

166 Let \mathbf{y}_k^j be the experimental results for replicate k for a given test j . For instance,
167 \mathbf{y}_1^j , \mathbf{y}_2^j , and \mathbf{y}_3^j can be the measured forces for three replicates of a three-point bending
168 test denoted j . In order to compare the experimental data, one needs at some point to
169 compute the arithmetic difference between experimental data and model response \mathbf{Y}_k^j as
170 $\boldsymbol{\varepsilon}_k^j = \mathbf{y}_k^j - \mathbf{Y}_k^j$. This expression implies that a model response, which depends on the given
171 spatial distribution of particles, corresponds to a specific replicate of the experimental test.
172 This is not entirely correct since the internal structure of the experimentally tested material
173 is only statistically replicated by the model.

174 To overcome this problem, a solution consists in: (i) averaging the experimental results
175 of all replicates to obtain the mean data \mathbf{y}^j , (ii) running multiple simulations with different
176 spatial distributions of particles and averaging the model responses to get \mathbf{Y}^j , and (iii)
177 comparing the experimental and numerical results in terms of mean responses. In this
178 process, there is a loss of information since the variance of the data is not known. Such a
179 task would require the use a true stochastic model which appears unnecessary with respect
180 to the very good results presented in Section 5. In addition, this loss remains minimal as the
181 interest in this work is on central range statistics, viz. mean values for normally distributed
182 regression errors, and is reduced as the number of replicates increases.

183 *3.2. Parameter estimation*

184 Let \mathbf{x}^j be the predictor variable, for instance the displacements corresponding to the
 185 forces \mathbf{y}^j or \mathbf{Y}^j . One can first discretize in equally spaced intervals the predictor variable
 186 over its range of values and define x_i^j , y_i^j , and Y_i^j at index $i = 1, \dots, n^j$ where n^j is the
 187 number of discretized points. Next, if one denotes f^j the model response corresponding to
 188 the simulation of test j and $\boldsymbol{\theta} = [\theta_1 \dots \theta_p]^t$ the parameter vector containing the p unknown
 189 model parameters to be estimated, then, $Y_i^j = f^j(x_i^j, \boldsymbol{\theta})$. Next, one can formulate the general
 190 minimization problem as follows:

$$\text{Find the least square estimate } \hat{\boldsymbol{\theta}} \text{ which minimizes } S^j = \sum_{i=1}^{n^j} (y_i^j - f^j(x_i^j, \boldsymbol{\theta}))^2 \quad (6)$$

191 where S^j is the residual sum of squares for curve j . Using the least-square method is here
 192 well justified as the conditional variance of the data used later on can be considered uniform
 193 and because the residuals of the regression $\varepsilon_i^j = y_i^j - f^j(x_i^j, \boldsymbol{\theta})$ can be generally assumed
 194 independent or non-correlated.

195 In the case of a single test, i.e. $j = 1$, the formulas stated earlier can be directly applied
 196 and S^1 can be minimized to obtain $\hat{\boldsymbol{\theta}}$. When multiple tests are considered simultaneously
 197 in the parameter identification process, one needs to normalize the residual sum of squares
 198 for each test and generate a global objective function to be minimized. This can be done by
 199 defining a new residual ϕ^j for each test j as follows:

$$\phi^j = \frac{S^j}{\sum_{i=1}^{n^j} (y_i^j)^2} \quad (7)$$

200 It is interesting to note that the normalization in Equation 7 becomes the Mean Absolute
 201 Percentage Error (MAPE) in the case of a single point estimate ($i = n^j = 1$).

202 The global residual is defined as a linear combination of ϕ^j for different tests j , which is
 203 consistent with the additive property of the square of the coefficient of variation of errors
 204 defined in Section 3.3. The general minimization problem is written as follows:

$$\text{Find the least square estimate } \hat{\boldsymbol{\theta}} \text{ which minimizes } \psi = \sum_{j=1}^N w^j \phi^j \quad (8)$$

205 where w^j can be seen as the weights for each test j and take the values between 0 and 1
 206 such that $\sum_{j=1}^N w^j = 1$. N is the total number of tests considered. In absence of specific
 207 information about the tests, one can assume equal weights, i.e. $\forall j, w^j = 1/N$.

208 3.3. Fit and prediction quality

209 Once the estimate $\hat{\theta}$ is obtained, one can appreciate the fit and prediction quality for
 210 each individual test. For this purpose, two statistical indicators are introduced and will be
 211 used throughout the paper.

212 The first indicator is the coefficient of variation of the regression errors ω^j which char-
 213 acterizes the ratio of the scatter band width to the data mean

$$\omega^j = \frac{s^j}{\bar{y}^j} \text{ where } s^j = \sqrt{\frac{S^j}{n^j - p}} \quad (9)$$

214 s^j is the standard error of the regression, $n^j - p$ is called degrees of freedom, and $\bar{y}^j =$
 215 $(\sum_{i=1}^{n^j} y_i^j) / n^j$ is the data mean.

216 The second one is the adjusted $(r^2)^j$, also called the coefficient of determination which
 217 characterizes the ratio of the scatter band width to the overall spread of data and indicates
 218 what percentage of data variation is accounted for by the model response. By defining the
 219 corrected total sum of squares $S_c^j = \sum_{i=1}^{n^j} (y_i^j - \bar{y}^j)^2$ and the standard deviation of all data
 220 $\bar{s}^j = \sqrt{S_c^j / (n^j - 1)}$, this indicator is written as:

$$(r^2)^j = 1 - \frac{(s^j)^2}{(\bar{s}^j)^2} \quad (10)$$

221 In the case of a single point estimate, i.e. $i = n^j = 1$, the aforementioned indicators
 222 are not valid. One can instead use the mean absolute percentage error which is written as
 223 $\text{MAPE}^j = 100|\varepsilon^j / y^j|$ where $\varepsilon^j = y^j - f^j(x^j, \hat{\theta})$, $y^j = y_1^j$ and $x^j = x_1^j$.

224 In order to evaluate and quantify an overall quality of fit and predictions, one simply
 225 needs to regroup all data points for each test with their corresponding model responses into
 226 one global set and compute the overall coefficient of variation of errors, ω , and the overall
 227 coefficient of determination, r^2 .

228 Let us underline that the coefficient of variation and the coefficient of determination are
229 mathematically derived for linear model regression only and are, in theory, not valid when
230 one performs regression or assesses quality of fit for non-linear (parameter-wise) models.
231 Nevertheless, they are often used in practice because of the absence of clear indicator for
232 quality of fit, aside from the standard error of regression which however is unit-dependent,
233 is not expressed in percentage, and is not bounded. In addition, one might argue that when
234 the model is already fitted and the problem is well-conditioned, the residual sum of squares
235 which is originally non-linear can be linearized around the least square estimate. Therefore,
236 close enough to the estimate and when the original and linearized residual sums of squares
237 are close enough, the use of these statistical indicators can be justified.

238 **4. Modeling and calibration process**

239 *4.1. Summary of experimental campaign*

240 In the experimental work by Grégoire et al. (2013), four sizes of geometrically similar
241 prismatic specimens with four depths $D = 50$ mm, 100 mm, 200 mm, and 400 mm, the
242 span-to-depth ratio S/D of 2.5, and the out-of-plane thickness of 50 mm were tested in
243 three-point bending. Unnotched and notched samples with a notch length a and the notch-
244 to-depth ratios $\alpha = a/D = 0.5, 0.2, 0$ were tested under CMOD control to obtain a stable
245 post-peak response. In the case of unnotched beams, the legs of the extensometer were
246 attached to the bottom surface of the beams at a distance from mid-span of half the beam
247 depth to ensure crack initiation between the legs. Splitting tests on cylinders were also
248 conducted to estimate tensile strength. In complement to fracture tests, cylindrical samples
249 were tested under unconfined compression and measurements of elastic parameters and
250 compressive strength were obtained. More details on the experimental program are given
251 by Grégoire et al. (2013).

252 *4.2. LDPM internal geometry*

253 The parameters required to construct the LDPM geometry were first identified based on
254 the actual mix design used in the experiments. The particle size distribution was numerically

255 reproduced following the procedure described in Yang et al. (2022) with a cut-off size $d_0 = 4$
 256 mm and a maximum size $d_a = 10$ mm. Figure 2(a) shows the experimental and numerical

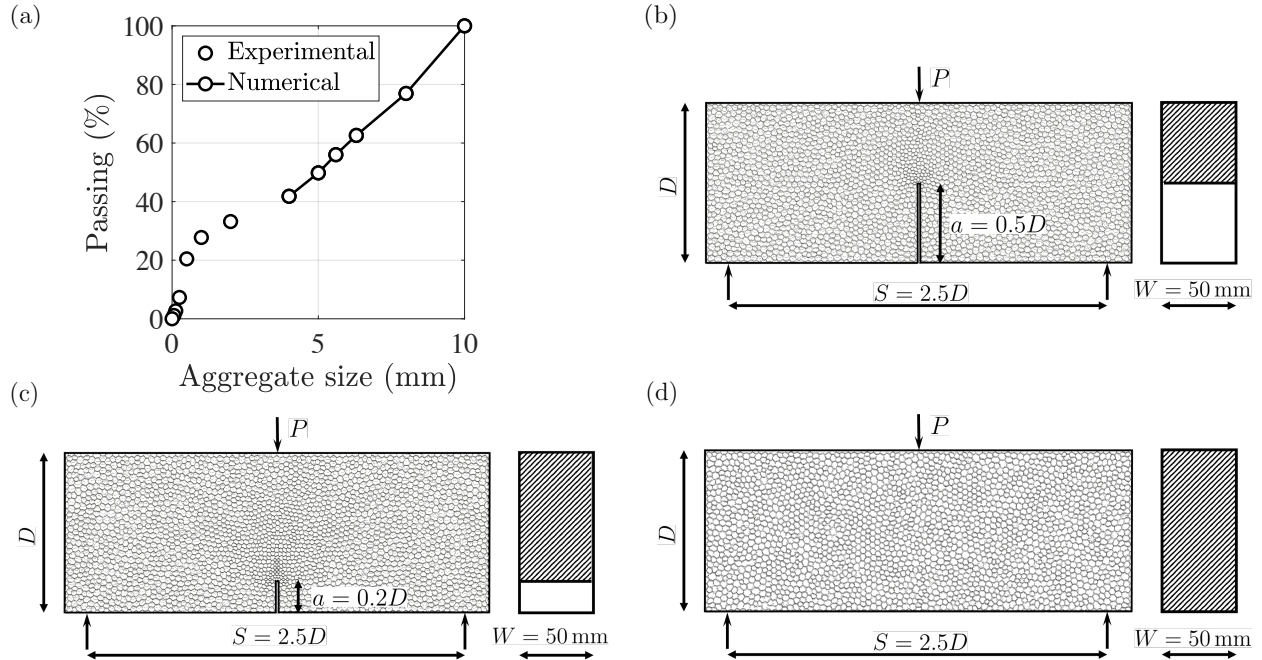


Figure 2: (a) Simulated particle size distribution, LDPM cells, geometries, and dimensions of the simulated beams with the notch-to-depth ratios of (b) 0.5, (c) 0.2, and (d) 0 viz. unnotched beam, for $D = 50$ mm, 100 mm, 200 mm, and 400 mm.

256
 257 sieve curves. The remaining parameters were also chosen based on the mix design: cement
 258 content $c = 286 \text{ kg m}^{-3}$, water-to-cement ratio $w/c = 0.626$, and density $\rho = 2121 \text{ kg m}^{-3}$.
 259 Figure 2(b)-(d) show the simulated geometries and the resulting LDPM cells at the surface
 260 of the samples.

261 4.3. Modeling and calibration process

262 The identification of the parameters in the constitutive laws describing elastic, tension,
 263 and tension-shear behaviors followed a two-step procedure. First, the normal modulus E_0
 264 and α_0 related to the elastic behavior were calculated using the approximated formulas listed
 265 in Section 2.2, based on the mean values of the macroscopic elastic modulus and Poisson's
 266 ratio reported by Grégoire et al. (2013). The values of $E_0 = 57180 \text{ MPa}$ and $\alpha_0 = 0.25$ were
 267 obtained.

268 Next, the three parameters related to fracture and shear, i.e. the mesoscale tensile
269 strength σ_t , the mesoscale fracture energy G_t , and the shear-to-tensile strength ratio r_{st} were
270 identified simultaneously based on: (i) the compressive strength obtained from cylinders
271 with the diameter $D_c = 74$ mm and the height $H_c = 142$ mm, and (ii) the entire load-
272 CMOD curve corresponding to the medium size beam with the depth $D = 200$ mm and
273 $\alpha = 0.2$. For the compression test, rigid plates were used on the top and bottom of the
274 specimens. Friction between the plates and the sample was simulated through a simple
275 Coulomb friction law with a friction coefficient $\mu = 0.13$. Concerning the bending test, the
276 loads were applied directly on the surface nodes. Both compression and fracture tests were
277 simulated under displacement control with a constant velocity of 1 mm s^{-1} to ensure quasi-
278 static conditions. For each test, three simulations were performed with different spatial
279 distributions of particles. The least square estimate of the parameter vector $\boldsymbol{\theta} = [\sigma_t \ G_t \ r_{st}]^t$
280 was obtained by minimizing the overall residual $\psi = \phi^C + \phi^{3\text{PBT}}$ where ϕ^C and $\phi^{3\text{PBT}}$ are the
281 residuals computed through Equation 7 for the compression and three-point bending tests,
respectively. The values of $\sigma_t = 2.9 \text{ MPa}$, $G_t = 45.5 \text{ N m}^{-1}$, and $r_{st} = 3.276$ were obtained.

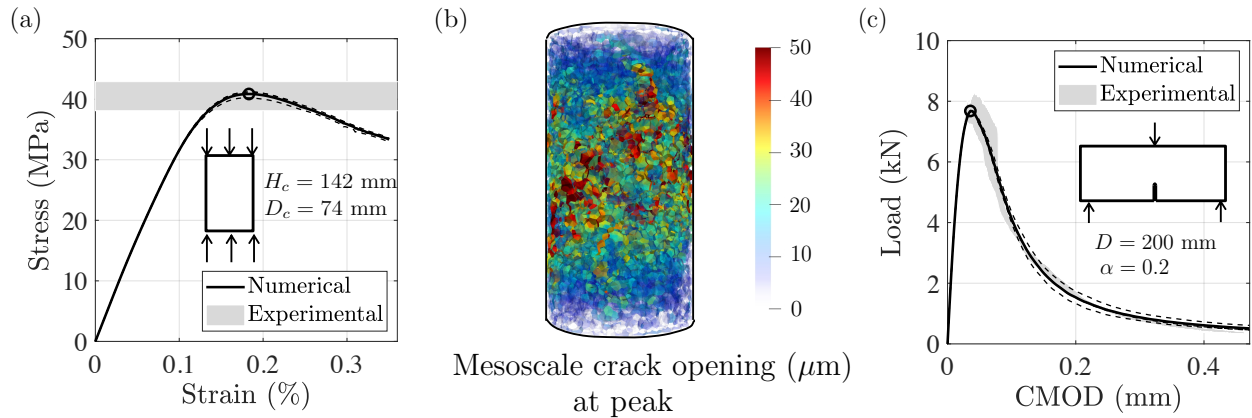


Figure 3: Calibration results: (a) stress-strain curve of the unconfined compression test on the cylinder with the diameter $D_c = 74$ mm and height $H_c = 142$ mm; the empty circle designates the mean peak value, (b) failure mode at the peak load (c) load-CMOD curve of the three-point bending test on the notched beam with $D = 200$ mm and $\alpha = 0.2$.

282
283 Figure 3(a) shows the simulated stress-strain curve of the compression test together
284 with the compressive strength obtained experimentally. The solid line is the mean curve of

285 the three individual simulations represented by dashed lines. The gray area represents the
 286 experimental scatter where the upper and lower bounds of the envelope corresponds to the
 287 maximum and minimum values of loads, respectively. The mode of failure at peak is shown
 288 in Figure 3(b), characterized by a shear band. The LDPM facets are colored according to the
 289 value of the mesoscale crack opening defined as $w = (w_N^2 + w_M^2 + w_L^2)^{\frac{1}{2}}$ for $e_N > 0$ and $w = 0$
 290 for $e_N < 0$, $w_i = l e_i^{ine}$ where $e_i^{ine} = e_i - t_i/E_i$ is the inelastic strain for $i = N, M, L$, and l
 291 is the edge length defined in Section 2.2. Figure 3(c) shows the experimental and numerical
 292 load-CMOD curves for the bending test. Typical failure modes are depicted in Figures 5(d),
 293 (e), (g) and (h). One can observe that the numerical results fit well the experimental data.
 294 In terms of quality of fit, a MAPE of 3.4% was reached for the compression test, whereas
 295 the three-point bending test fit was characterized by a coefficient of variation $\omega = 6.8\%$ and
 296 a coefficient of determination $r^2 = 0.995$. It is interesting to note that the ratio between
 297 the macroscopic splitting tensile strength f_{st} reported in Section 5.1 and the compressive
 298 strength f'_c shown in Figure 3(a) is approximately 9%, which is consistent with the range of
 299 values reported in the literature. Note also that the mesoscale tensile strength σ_t and the
 300 compressive yielding strength σ_{c0} are not macroscopic properties but only model parameters.

301 As explained in Section 2, concrete failure is characterized by multiple mechanisms that
 302 are different and LDPM is able to simulate all these mechanisms. For each mechanism,
 303 there is a set of relevant model parameters (less than 4) which makes the total number of
 304 parameters to be 16. The elastic behavior modeled by two parameters (E_0, α_0) and the
 305 mesoscale mixed mode fracture governed by three parameters (σ_t, G_t, r_{st}) have been identi-
 306 fied. The remaining parameters were assumed based on the actual mix design and Section
 307 5.3 by Cusatis et al. (2011b), namely the softening exponent n_t governing the interaction
 308 between shear and tensile behavior during softening, ($\sigma_{c0}, H_{c0}, \kappa_{c0}, E_d$) defining the behavior
 309 of the facet normal component under compression and affecting the macroscopic behavior in
 310 compression, ($\mu_0, \mu_\infty, \sigma_{N0}$) contributing to the LDPM response in compression, mainly the
 311 triaxial compressive behavior at high-confinement, (κ_{c1}, κ_{c2}) governing the nonlinear evolu-
 312 tion of the normal facet stress in compression, and finally β controlling the coupling between
 313 the mesoscale compressive behavior and the macroscopic triaxial compressive behavior. All

314 parameters are listed in Table 1 for the sake of clarity.

Table 1: Values of the material model parameters used in the numerical simulations

Designation	Symbol	Units	Value	Source
Density	ρ	kg m ⁻³	2338	Grégoire et al. (2013)
Water-to-cement ratio	w/c	-	0.626	Grégoire et al. (2013)
Maximum aggregate size	d_a	mm	10	Grégoire et al. (2013)
Minimum aggregate size	d_0	mm	4	Fixed
Effective normal modulus	E_0	MPa	57,180	Identified
Shear-normal coupling parameter	α_0	-	0.25	Identified
Tensile strength	σ_t	MPa	2.9	Identified
Fracture energy	G_t	N mm ⁻¹	45.5	Identified
Shear strength ratio	r_{st}	-	3.276	Identified
Softening exponent	n_t	-	0.2	Cusatis et al. (2011b)
Compressive yielding strength	σ_{c0}	MPa	120	Cusatis et al. (2011b)
Initial hardening modulus ratio	H_{c0}/E_0	-	0.4	Cusatis et al. (2011b)
Transitional strain ratio	κ_{c0}	-	2	Cusatis et al. (2011b)
Deviatoric strain threshold ratio	κ_{c1}	-	1	Cusatis et al. (2011b)
Deviatoric damage parameter	κ_{c2}	-	5	Cusatis et al. (2011b)
Initial friction	μ_0	-	0.2	Cusatis et al. (2011b)
Asymtotic friction	μ_∞	-	0.0	Cusatis et al. (2011b)
Transitional stress	σ_{N0}	MPa	600	Cusatis et al. (2011b)
Densification ratio	E_d/E_0	-	1.0	Cusatis et al. (2011b)
Volumetric deviatoric coupling	β	-	0.0	Cusatis et al. (2011b)

315 5. Prediction results and discussion

316 The capability of the model to simulate fracture and predict size-effect was assessed by
317 carrying out blind simulations, i.e. without adjusting model parameters, on splitting and
318 size-effect tests for different beam sizes and notch lengths.

319 *5.1. Splitting test*

320 LDPM was first validated on splitting tests for which peak loads for nine replicates are
 321 reported by Grégoire et al. (2013). For this purpose, three cylinders with the height $L_s = 215$
 322 mm and the diameter $D_s = 113$ mm with different spatial distributions of particles were
 323 simulated. The load was applied directly on particles at the surface of the cylinder. In
 324 addition, the simulations were performed under displacement control with a constant loading
 325 rate of 1 mm s^{-1} to ensure quasi-static conditions.

326 Figure 4(a) shows the mean predicted nominal stress versus displacement curve repre-
 327 sented by a solid line and the three individual simulations in dashed lines, along with the
 experimental scatter represented with a gray area. The nominal strength was computed

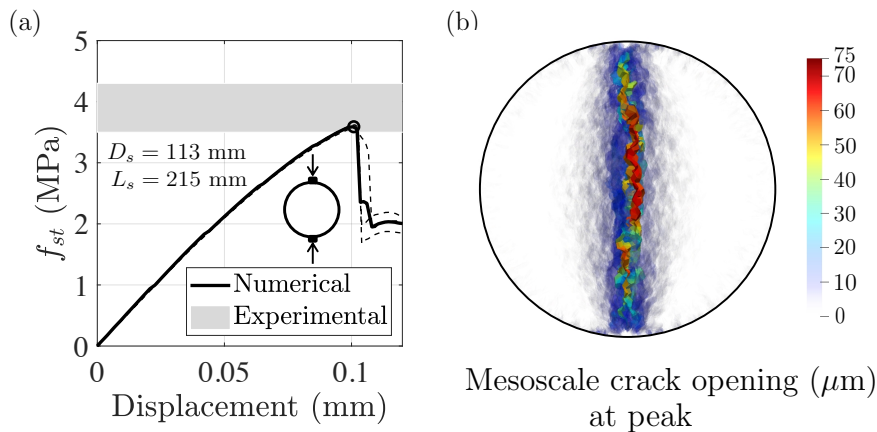


Figure 4: Prediction results: (a) nominal stress-displacement curve of the splitting test; the empty circle designates the mean peak value, and (b) failure mode at the peak load.

328 using the formula $f_{st} = (2P_{st,u})/(\pi D_s L_s)$ where $P_{st,u}$ is the splitting peak force. One can
 329 observe that the numerical mean splitting tensile strength is within the scatter of the exper-
 330 iments. A MAPE of 7.5% was found when comparing the experimental and simulation peak
 331 values, which indicates a good accuracy in the prediction with respect to the scatter observed
 332 in experiments. Figure 4(b) shows the mode of failure at the peak load. As expected and
 333 in accordance with experimental observation, fracture initiates at the center where tensile
 334 stresses are the highest. The main crack is tortuous and has a slight eccentricity with respect
 335 to the vertical line passing through the center. This is due to the inherent ability of the
 336

337 mesoscale model to reproduce heterogeneity in the material, and is by the way routinely
338 observed in experiments (Rocco, 1996; Bažant and Planas, 1997).

339 *5.2. Size-effect tests*

340 *5.2.1. Load-CMOD curves*

341 The model was next used to predict the load-CMOD curves for all sizes and notch
342 lengths. The simulations were performed under displacement control and quasi-staticity was
343 ensured by applying loads at a constant loading rate of 1 mm s^{-1} . Figures 5(a)-(c) show the
344 predicted curves for the notch-to-depth ratios of 0.5, 0.2, and 0, respectively. The solid line
345 is the mean response of the three individual simulations in dashed lines. The experimental
346 scatter is represented with a gray area. One can observe that the numerical simulations
347 predict well the mechanical behavior in the elastic, near-peak and post-peak regimes for the
348 different geometries and sizes. The prediction in the post-peak of the smallest size beam
349 with a notch-to-depth ratio of 0.5 deviates from the experimental results. The reason might
350 be that the number of aggregates in the ligament is not enough and makes the model too
351 coarse. In addition, boundary effects play a significant role for such small specimens. In the
352 case of the two unnotched beams with largest sizes, the response stops at the peak due to
353 snapback, similarly to what was observed in the experiments.

354 *5.2.2. Fracture process zone and dissipated energy*

355 Figures 5(d)-(i) show the typical failure modes for the beams with the size $D = 100$
356 mm for two different displacement values. Two types of failure can be distinguished. (i)
357 For the notched specimens, the FPZ is localized and emanates at the crack tip. It develops
358 for the increasing load and finally reaches an ultimate size at the peak load (Figures 5(d)
359 and (e)). The FPZ of the constant size then propagates through the ligament (Figures 5(g)
360 and (h)), which explains the strain softening behavior observed at the macroscale. (ii) For
361 the unnotched specimens, the FPZ initiates at the bottom surface of the sample, where the
362 stresses approach the material tensile strength, and is diffused on a zone much larger in size as
363 compared to the notched-beam case. As the load increases up to the peak, the damaged zone

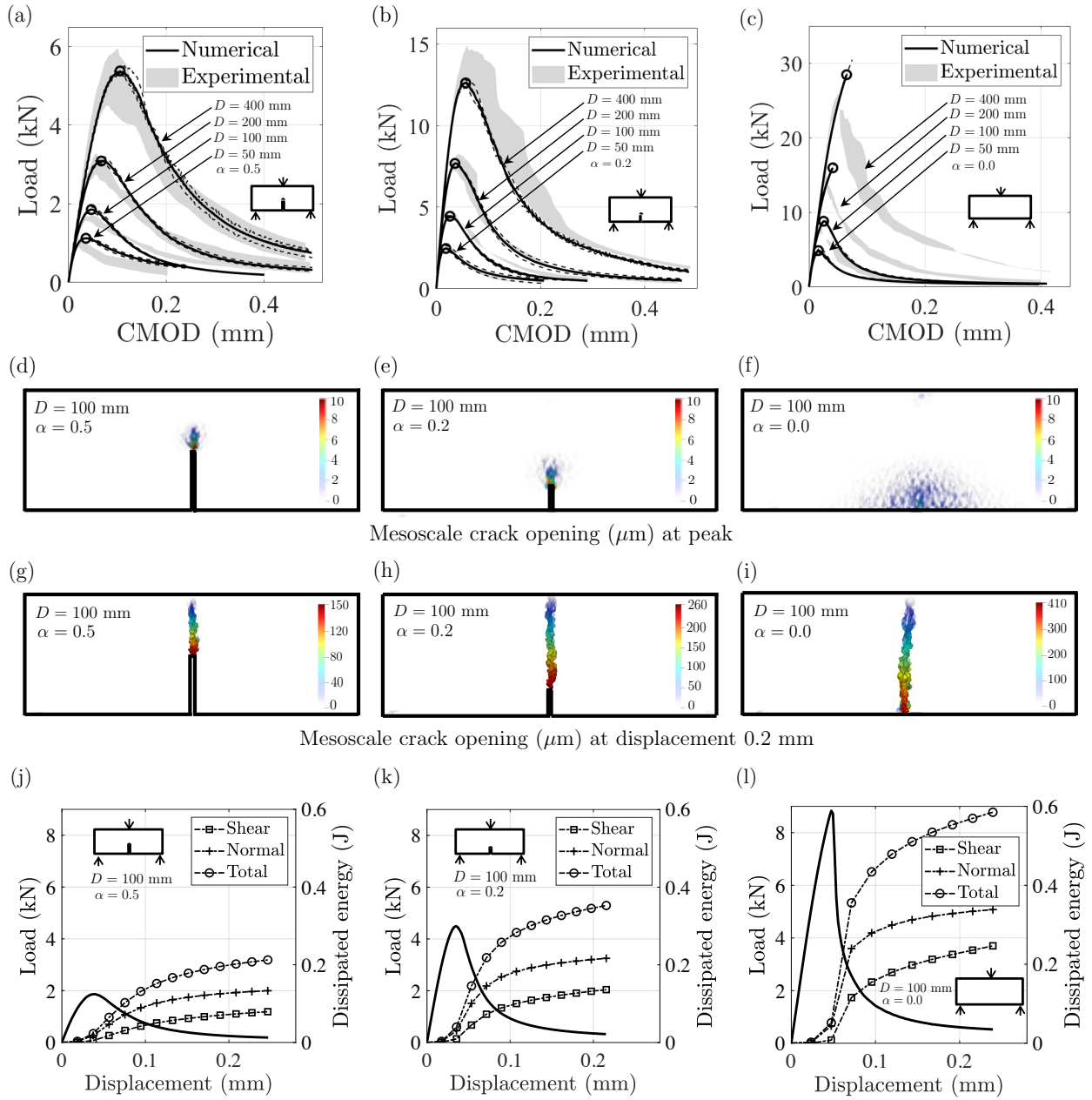


Figure 5: Prediction results: load-CMOD curves for (a) $\alpha = 0.5$, (b) $\alpha = 0.2$, (c) $\alpha = 0$, the empty circles designate mean peak values; failure modes at the peak load for the samples with the depth $D = 100$ mm for (d) $\alpha = 0.5$, (e) $\alpha = 0.2$, (f) $\alpha = 0$; failure modes at a displacement of 0.2 mm for the samples with the depth $D = 100$ mm for (g) $\alpha = 0.5$, (h) $\alpha = 0.2$, (i) $\alpha = 0$; dissipated energies for (j) $\alpha = 0.5$, (k) $\alpha = 0.2$, (l) $\alpha = 0$.

364 becomes larger (Figure 5(f)). At the peak load, the FPZ eventually collapses to a single crack
365 that propagates, whereas the surrounding strained material unloads. One can also observe
366 that the final crack does not necessarily originate at mid-span. This phenomena shows
367 the direct effect of material heterogeneity, realistically captured by the mesoscale model.
368 Although not quantified here, the evolution of the FPZ is consistent with the one described
369 in Lefort et al. (2015) based on Ripley's function analysis on the same experimental data.

370 As a matter of fact, the very nature of the model allows one to assess shear and tensile
371 behaviors during fracture propagation in contrast with continuum models where smear cracks
372 over a region and are unable to capture local oriented events. In general, the LDPM facets
373 are subject to both tensile and shear strains even though the test configuration is designed
374 for mode I opening. One can look at the evolution of the dissipated energy computed from
375 the increment of the dissipated energy density $\dot{w}_d = 3(t_N \dot{e}_N^{ine} + t_M \dot{e}_M^{ine} + t_L \dot{e}_L^{ine})$ for $e_N > 0$
376 and the volume of the cell I containing the facet $V_I = (\sum_k A_k^p l_k)/3$. Summing over the entire
377 volume of the sample, one can obtain the evolution in time (or displacement here) of the total
378 dissipated energy W_d and dissociate the individual contributions of the normal component
379 $W_{d,N}$ and the tangential components $W_{d,T}$. In the present simulations, $W_{d,N}$ almost coincides
380 with the energy dissipated in tension. Figures 5(j)-(l) show the load-displacement curves
381 for the beams with the size $D = 100$ mm for the three different notch lengths, together
382 with the dissipated energies. As expected, the total energy dissipated at the end of the
383 test/simulation is smaller for the larger notch length, i.e. for a smaller ligament length.
384 This is consistent with the acoustic energy obtained from acoustic emission on the same
385 type of experiments reported in the work of Grégoire et al. (2015).

386 Moreover, one can observe a sharper increase in the dissipated energy as the notch length
387 decreases, which is consistent with the increase in brittleness as α tends to zero. Up to the
388 peak load, the energy dissipated in shear is negligible as compared to the one in tension,
389 for all cases including the unnotched beam. However in the post-peak regime, the energy
390 dissipated in shear becomes more than half of the energy dissipated in tension, which proves
391 that the post-peak behavior involves both shear and tensile forces in the meso-structure.

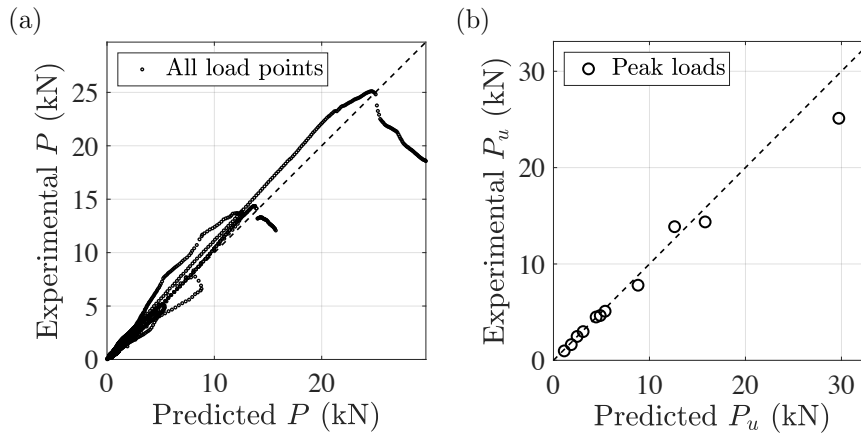


Figure 6: Statistics of the model predictions: (a) scatter of the measured versus predicted values of loads, and (b) scatter of the measured versus predicted values of the peak loads only. The dashed lines correspond to the 1:1 lines.

393 The quality of predictions was also assessed. Figure 6(a) shows the scatter between ex-
 394 perimental and numerical loads for all geometries and sizes, on the entire load-displacement
 395 curves. Figure 6(b) shows the same scatter but only for the peak values. In both figures,
 396 the cloud of points are close to the 1:1 lines. The set of load points that deviate the most
 397 to the 1:1 lines corresponds to the largest unnotched beam (Figure 6(a)). The prediction
 398 overestimates the peak load by about 15% (Figure 6(b)). One might be tempted to invoke
 399 statistical size-effect related to the randomness in material properties, which is not captured
 400 by the deterministic version of LDPM used in this study. Such an effect can be effectively
 401 simulated by introducing random fields on the mesoscale model parameters as performed in
 402 the work of Eliáš and Vořechovský (2020). Nevertheless, the deterministic predictions are
 403 inaccurate only for the unnotched beam of size $D = 400$ mm. Further testing on larger
 404 unnotched beam sizes would help validate or invalidate a possible statistical effect for beam
 405 with the size $D = 400$ mm. In addition, the use of random fields would add a new level
 406 of complexity by making the inverse parameter identification problem ill-conditioned with
 407 respect to the limited reported experimental data.

408 Overall, a coefficient of determination of $r^2 = 0.94$ and a coefficient of variation of

409 $\omega = 36.8\%$ were found when all load points are considered. For the peak loads only, the
410 values of $r^2 = 0.95$ and $\omega = 23.5\%$ were obtained. The values of the coefficients of variation
411 show that the numerical predictions are very reasonable and are within the typical scatter
412 observed in concrete fracture testing. These results demonstrate quantitatively the capability
413 of the model to predict the effects of size and geometry during concrete failure.

414 *5.3. Universal size-effect law and fracture parameters*

415 Macroscopic properties of concrete such as compressive or tensile strength are usually
416 determined in laboratory using standardized sample dimensions. On the other hand, size-
417 effect tests applied in a certain range of sizes were shown to provide an accurate estimation of
418 fracture properties (RILEM, 1990). This method is preferred to the work of fracture method
419 that provides apparent fracture properties which are geometry and size dependent. The size-
420 effect method only requires the knowledge of peak loads and sample geometry (Bažant and
421 Planas, 1997). It appears therefore interesting to compare the fracture parameters obtained
422 using experimental results as reported by Grégoire et al. (2013) and parameters one could
423 identify using the numerical predictions, keeping in mind that only one load-CMOD curve
424 on a single size notched beam was sufficient for model calibration.

425 For this purpose, many approximated formulae exist and can be used (Morel, 2008;
426 Cusatis and Schaufert, 2009; Bažant and Yu, 2009; Di Luzio and Cusatis, 2018; Chen and
427 Hu, 2022). Typically, two parameters are enough to capture size-effect in notched three-
428 point bending tests (RILEM, 1990; Planas et al., 1997; Cusatis and Schaufert, 2009; Chen
429 and Hu, 2022). Unnotched specimens can also be simulated but the size cannot be too
430 large as statistical size-effect becomes non-negligible (Eliáš et al., 2015). In this study,
431 the so-called Universal Size Effect Law (USEL) in its deterministic version (Bažant and
432 Yu, 2009) was considered. This fitting formula bridges Type I size-effect which occurs in
433 structures that fail at crack initiation from a smooth surface and Type II size-effect occurring
434 in notched structures. It also covers the two distinct asymptotic behaviors at large size in
435 the typical double-logarithm nominal strength versus structural size representation: (i) 1/2
436 slope corresponding to linear elastic fracture mechanics for Type II size-effect and (ii) a

437 straight horizontal line corresponding to the elastic limit for Type I size-effect. The formula
 438 is written as:

$$\sigma_{Nu} = \sqrt{\frac{EG_f}{g'_0 c_f + g_0 D} \left(1 - \frac{r c_f^2 g''_0 e^{-k\alpha^2}}{4(l_p + D)(g_0 D + g'_0 c_f)} \right)^{1/r}} \quad (11)$$

439 where $\sigma_{Nu} = (3P_u S)/(2WD^2)$ is the nominal strength corresponding to the peak load P_u ,
 440 G_f is the fracture energy, and c_f is the effective length of the FPZ. $g_0 = g(\alpha_0)$ is the
 441 dimensionless energy release rate, and $g'_0 = g'(\alpha_0)$ and $g''_0 = g''(\alpha_0)$ are its first and sec-
 442 ond derivatives, respectively, evaluated at the initial notch-to-depth ratios $\alpha_0 = 0.5, 0.2, 0$.
 443 Finally, r , k , and l_p are empirical constants. Based on the expression of $g(\alpha)$ reported for
 444 example by Bažant and Planas (1997) or Grégoire et al. (2013), the following values were
 445 computed for the geometry studied in this paper: $g_0 = 2.96$, $g'_0 = 18.95$, and $g''_0 = 153.88$
 446 for $\alpha = 0.5$, $g_0 = 0.57$, $g'_0 = 3.17$, and $g''_0 = 10.77$ for $\alpha = 0.2$, and $g_0 = 0$, $g'_0 = 3.41$, and
 447 $g''_0 = -16.75$ for $\alpha = 0$. By keeping the empirical constants $r = 0.11$, $k = 113$, and $l_p = 12.9$
 448 identical to the ones reported in the work of Grégoire et al. (2013), the model was fitted
 449 using the simulation data. The values of the fracture energy and effective length, $G_f = 39$
 450 N m^{-1} and $c_f = 16.8$ mm were obtained with a coefficient of determination $r^2 = 0.97$ and a
 451 coefficient of variation of $\omega = 1.82\%$. Figures 7(a)-(b) show the fitted model plotted together
 452 with the experimental and numerical data.

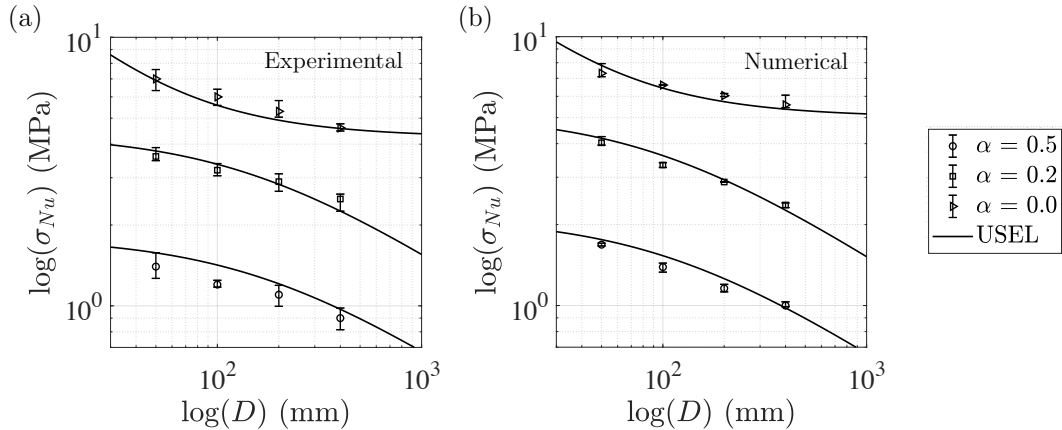


Figure 7: Fitting with the Universal Size Effect Law: nominal strength versus size for (a) experimental data and (b) simulation results.

453 These predicted fracture parameters are to be compared with the ones identified using

454 the experimental results, i.e. $G_f = 42.6 \text{ N m}^{-1}$ and $c_f = 25.7 \text{ mm}$ (Grégoire et al., 2013):
455 both fracture energy and effective length can be qualitatively considered close enough with
456 respect to the scatter of typical experiments on concrete. This result suggests that one could
457 perform only one fracture test on a specific geometry in the laboratory, calibrate and use
458 LDPM to simulate different sizes (and possibly geometries) to finally identify the fracture
459 energy and effective length of the FPZ through a size-effect law.

460 6. Conclusions

461 In this study, a large set of experimental results on fracture and size-effect including
462 the effect of geometry was simulated using the Lattice Discrete Particle Model (LDPM).
463 The load-CMOD curve of a single size notched beam under three-point bending, and the
464 compressive strength were used for model calibration. The remaining experimental results,
465 namely one splitting test and eleven three-point bending tests of different beam sizes and
466 notch lengths, were used for model validation without parameter adjustment. The fracturing
467 process was discussed along with a rigorous quantification of quality of fit and quality of
468 predictions. Fracture parameters using the numerical results were identified through the
469 Universal Size Effect Law (USEL). Based on the obtained results the following conclusions
470 can be drawn:

- 471 • The compressive strength and the load-CMOD curve of a single notched beam size are
472 sufficient for a complete model calibration in elastic, tensile and tensile-shear behaviors.
- 473 • The predictions on splitting tests and on the different beam geometries and sizes are
474 overall in excellent agreement with the experimental data.
- 475 • The fracturing process is well captured by LDPM for both notched and unnotched
476 beams.
- 477 • The dissipated energy in shear constitutes a large part of the total dissipated energy
478 in the post-peak.

479 • The fracture energy can be estimated through a size-effect law by using the simulation
480 results.

481 • The use of a stochastic model does not seem to be justified with respect to the limited
482 range of beam sizes.

483 7. Declarations of interest

484 The Authors declare that there is no conflict of interest.

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492 9. Appendix

493 9.1. LDPM constitutive equations for pore collapse, compaction, and frictional behavior

494 The pore collapse and material compaction occur for $e_N < 0$. Strain hardening plas-
495 ticity behavior due to high compressive hydrostatic deformation is computed through a
496 strain-dependent boundary $\sigma_{bc}(e_D, e_V)$ at each facet which limits the normal compressive
497 stress component via the inequality $-\sigma_{bc}(e_D, e_V) \leq t_N \leq 0$, in which the volumetric
498 strain is defined as $e_V = \Delta V / (3V_0)$, computed as the change between the current and
499 the initial volume of each LDPM tetrahedron. While e_V is the same for all the facets
500 of a given tetrahedron, the deviatoric strain defined as $e_D = e_N - e_V$ changes. Finally,
501 the strain-dependent boundary is calculated for three different cases $\sigma_{bc}(e_D, e_V) = \sigma_{c0}$ for
502 $-e_V \leq 0$, $\sigma_{bc}(e_D, e_V) = \sigma_{c0} + \langle -e_V - \varepsilon_{c0} \rangle H_c(r_{DV})$ for $0 \leq -e_V \leq e_{c1}$ and $\sigma_{bc}(e_D, e_V) =$
503 $\sigma_{c1}(r_{DV}) \exp [(-e_V - e_{c1})H_c(r_{DV}) / \sigma_{c1}(r_{DV})]$ otherwise, where $r_{DV} = |e_D| / e_V$ for $e_V > 0$

504 and $r_{DV} = -|e_D|/(e_V - e_{V0})$ for $e_V \leq 0$ in which $e_{V0} = \kappa_{c3}e_{c0}$. $e_{c0} = \sigma_{c0}/E_0$ defines σ_{c0} the
 505 mesoscale yielding compressive stress, $e_{c1} = \kappa_{c0}e_{c0}$ is the strain at which the rehardening
 506 starts, κ_{c0} and κ_{c3} are material constants and $\sigma_{c1}(r_{DV}) = \sigma_{c0} + (e_{c1} - e_{c0})H_c(r_{DV})$. The
 507 function $H_c(r_{DV})$ reads as $H_c(r_{DV}) = H_{c1} + (H_{c0} - H_{c1})/(1 + \kappa_{c2}\langle r_{DV} - k_{c1} \rangle)$ where H_{c0} ,
 508 H_{c1} , κ_{c1} and κ_{c2} are material constants.

509 The frictional behavior due to compression-shear occurs also for $e_N < 0$. In the presence
 510 of compressive stresses, the shear strength increases due to frictional effects. The frictional
 511 behavior is simulated by means of a nonlinear Mohr-Coulomb model in which the internal
 512 friction coefficient varies from an initial value μ_0 to zero. The formulation can be written
 513 as $\sigma_{bs} = \sigma_s + \mu_0\sigma_{N0} - \mu_0\sigma_{N0} \exp(\sigma_N/\sigma_{N0})$ where σ_s is the cohesion stress and σ_{N0} is the
 514 transitional stress.

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