



Grassl, P. and Antonelli, A. (2019) 3D network modelling of fracture processes in fibre-reinforced geomaterials. *International Journal of Solids and Structures*, 156-57, pp. 234-242. (doi:[10.1016/j.ijsolstr.2018.08.019](https://doi.org/10.1016/j.ijsolstr.2018.08.019))

There may be differences between this version and the published version. You are advised to consult the publisher's version if you wish to cite from it.

<http://eprints.gla.ac.uk/168217/>

Deposited on: 4 September 2018

Enlighten – Research publications by members of the University of Glasgow
<http://eprints.gla.ac.uk>

3D network modelling of fracture processes in fibre-reinforced geomaterials

Peter Grassl^{*,1} and Adrien Antonelli^{1,2}

¹School of Engineering, University of Glasgow, UK

²Ecole Normale Supérieure Paris-Saclay, France

*Corresponding author: Email: peter.grassl@glasgow.ac.uk, Phone: +44 141 330 5208

Abstract

The width of fracture process zones in geomaterials is commonly assumed to depend on the type of heterogeneity of the material. Still, very few techniques exist, which link the type of heterogeneity to the width of the fracture process zone. Here, fracture processes in geomaterials are numerically investigated with structural network approaches, whereby the heterogeneity in the form of large aggregates and low volume fibres is modelled geometrically as poly-dispersed ellipsoids and mono-dispersed line segments, respectively. The influence of aggregates, fibres and combinations of both on fracture processes in direct tensile tests of periodic cells is investigated. For all studied heterogeneities, the fracture process zone localises at the start of the softening regime into a rough fracture. For aggregates, the width of the fracture process zone is greater than for analyses without aggregates. Fibres also increase the initial width of the fracture process zone and, in addition, result in a widening of this zone due to fibre pull out.

Keywords: fibres, fracture, geomaterial, heterogeneity, roughness

1 Introduction

Many structures made of geomaterials exhibit failure processes which are influenced by the heterogeneity of the material at an intermediate (meso-) scale. For instance, the type of coarse aggregates in concrete influences stiffness, strength and fracture energy of the material. For fibre reinforced cementitious materials, fibre type and geometry strongly influence the tail of the stress-crack opening curve (Naaman et al., 1991; Li and Wu, 2007). Therefore, modelling approaches which link the geometry, spatial distribution and mechanical properties of individual constituents at the meso-scale to the structural response are attractive. Furthermore, detailed investigations based on experiments and computational modelling of the mechanical interaction of individual constituents can contribute to further understanding of failure processes at larger scales.

Numerical approaches based on nonlinear fracture mechanics (NLFM) (Dugdale, 1960; Barenblatt, 1962) are commonly used to predict the failure of structural components of practical size, since the length of the fracture process zone is too large (with respect to the size of the structural component) for linear elastic fracture mechanics (LEFM), but too small for plastic limit load analysis to be applicable. Here, fracture process zone is defined as the zone in which energy is dissipated at a certain stage during the fracture process. Within computational frameworks, such as the finite element method and discrete stiffness approaches, NLFM is applied in the form of cohesive-crack and crack-band models. In cohesive-crack models, the displacement field across the fracture process zone is replaced by a displacement jump representing the crack opening and stresses are determined from a stress-crack opening law (Hillerborg et al., 1976; Carol et al., 1997). In crack-band models, the displacement jumps are transformed into cracking strains, so that the stress is calculated using stress-strain laws taking into account the size of the regions in which strains localise (Bažant and Oh, 1983). This size is usually a function of the element size, so that the load-displacement curves obtained with this approach are mesh-independent (Jirásek and Bauer, 2012). Discrete approaches describe both elastic and inelastic responses by means of force-displacement laws between discrete

49 bodies (Schlangen and van Mier, 1992a,b; Bolander et al., 2000). Often, these force-
50 displacement laws are chosen to be very similar to crack band approaches (Grassl and
51 Bolander, 2016). These different computational NLFM approaches can model the length
52 of the fracture process zone along the fracture, but not its width.

53 Continuum mechanics is an alternative to nonlinear fracture mechanics, where the frac-
54 ture process zone is represented by localised but regular fields of displacements. This
55 is achieved by including a length parameter in continuum models (Pijaudier-Cabot and
56 Bažant, 1987; Bažant and Jirásek, 2002). Maintaining a regularised displacement field
57 during fracture simulations provides mesh-independent solutions upon mesh refinement.
58 However, the length parameter influences the numerically predicted peak load and defor-
59 mation capacity of structures (Xenos and Grassl, 2016). Therefore, this parameter should
60 be chosen so that the localised field of displacements matches the width of the fracture
61 process zone of the material (Xenos et al., 2015).

62 The fracture process zone in heterogeneous materials such as concrete has been investi-
63 gated experimentally and numerically. Experimental studies for fracture in plain concrete
64 in Mihashi et al. (1991); Mihashi and Nomura (1996); Otsuka and Date (2000); Grégoire
65 et al. (2015) showed that the fracture process zone consists of a narrow band of high dis-
66 sipation surrounded by a wider region of low dissipation. Fracture surface measurements
67 were also performed to provide further insight into the link between roughness and frac-
68 ture behaviour (Lange et al., 1993; Mourot et al., 2006; Morel et al., 2008; Ponson et al.,
69 2006). In Grassl and Jirásek (2010); Grassl et al. (2012); Grégoire et al. (2015); Xenos
70 et al. (2015), information about the width of the fracture process zone is determined nu-
71 merically using two-dimensional structural network approaches for the meso-scale of plain
72 concrete consisting of coarse aggregates embedded in a mortar matrix. Numerical models
73 for fibre reinforced concrete, in which fibres were modelled discretely, were proposed in
74 Bolander and Saito (1997); Leite et al. (2004, 2007); Kabele (2007); Radtke et al. (2010);
75 Kunieda et al. (2011); Schaufert and Cusatis (2011); Caggiano et al. (2012); Montero-
76 Chacón et al. (2013); Kang et al. (2014); Zhan and Meschke (2016); Kang and Bolander

77 (2017); Montero-Chacón et al. (2017). Most of these studies on fibre reinforced composites
78 aimed at predicting the influence of fibres on stiffness, strength and ductility. There is
79 less information available on how fibres affect the spatial distribution of dissipated energy
80 at the meso-scale.

81 The aim of this work is to obtain more information about fracture processes in geoma-
82 terials at the meso-scale by using a three-dimensional structural network model. The
83 meso-structure of geomaterials is idealised to consist of a matrix with coarse aggregates,
84 interfacial transition zones (ITZs) between matrix and aggregates, and fibres. Periodic
85 direct tension analysis are performed and the effect of aggregates and fibres on the stress-
86 displacement curves and spatial distribution of energy dissipation are investigated.

87 **2 Method**

88 The present numerical approach for obtaining information on fracture processes in fibre-
89 reinforced quasi-brittle materials relies on periodic meso-structure generation, periodic
90 network modelling of the material response, and roughness evaluation of the fracture
91 patterns obtained from the network modelling. In the following sections, the individual
92 modelling techniques are described in more detail.

93 **2.1 Periodic meso-structure generation**

94 The meso-structure of concrete is modelled as coarse aggregates and fibres embedded
95 in a mortar matrix. Aggregates and fibres are idealised as poly-dispersed ellipsoids and
96 mono-dispersed line segments, respectively. They are periodically arranged in a compu-
97 tational cell representing the meso-structure of the material. For a given volume fraction
98 of ellipsoids, Fuller’s grading curve is used to determine the size distribution of ellipsoids
99 (Figure 1a). The total volume of ellipsoids is divided into intervals using sieve sizes. For
100 each volume interval, the upper and lower sieve sizes are m and $n = m/2$, respectively.

101 Here, m is smaller than or equal to the maximum sieve size $d_{a,\max}$ and n is greater than or
102 equal to the minimum sieve size $d_{a,\min}$. Starting with the volume interval obtained with
103 the largest pair of sieve sizes, ellipsoids are generated randomly with radii $s_3 > s_2 > s_1$
104 so that they fit through the square sieve size m , but not n (Figure 1b) as proposed in
105 Slowik and Leite (1999); Leite et al. (2007) and further investigated in Mehrotra (2011).
106 This results in the conditions

$$\frac{1}{2}\sqrt{\frac{2}{r^2+1}}rn < s_1 < \frac{1}{2}m \quad (1)$$

$$s_3 = s_1/r \quad (2)$$

$$\max\left(s_1, \sqrt{\frac{n^2}{2} - s_1^2}\right) \leq s_2 \leq \min\left(s_3, \sqrt{\frac{m^2}{2} - s_1^2}\right) \quad (3)$$

109 Here, r is uniformly distributed between 0.5 and 1. Furthermore, s_1 and s_2 are uniformly
110 distributed between the limits stated in (1) and (3), respectively. Line segments are
111 assumed to be of uniform length l_f . For a volume fraction ρ_f , the number of fibres are
112 calculated as $n_f = 4\rho_f V/(\pi d_f^2 l_f)$, where V is the volume of the unit cell and d_f is the
113 diameter of the fibres.

114 The input parameters for the meso-structure generation are the volume fraction of el-
115 lipsoids ρ_a , the maximum and minimum sieve sizes $d_{a,\max}$ and $d_{a,\min}$, respectively, the
116 volume fraction of line segments ρ_f , fibre length l_f and the diameter of fibres d_f . Only
117 ellipsoids greater than the sieve size $d_{a,\min}$ are generated, as indicated by the shaded region
118 in Figure 1a.

119 Next, ellipsoids and line segments are placed in the periodic cell by a random sequential
120 addition approach (Feder, 1980) so that the centroids of ellipsoids and line segments are
121 within the cell. Attention is paid so that the random orientation of ellipsoids and line
122 segments are uniformly generated within the volume (Muller, 1959). For every randomly
123 placed object, overlap with previously placed objects is checked. If overlap is avoided,
124 the object is placed in the cell and 26 mirror objects in the adjacent cells are generated
125 by shifting the object to the adjacent periodic cells. If overlap is detected, a new random

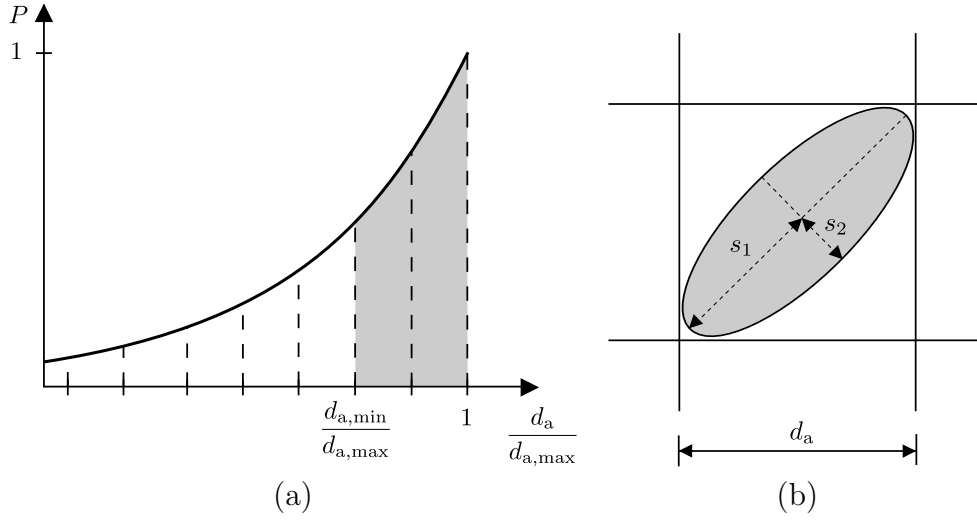


Figure 1: Generation of poly-dispersed ellipsoids (a) Sieve curve based on Fuller's curve and (b) geometrical restriction imposed by square sieve size.

126 position and orientation is generated. This process is repeated until all objects are placed
 127 in the cell. For the overlap check between ellipsoids, the algebraic system of equations in
 128 Wang et al. (2001) is used (Figure 2). Compared to the overlap check for spheres, solving
 129 this system of equations is slow. Therefore, outer and inner bounding spheres of the
 130 ellipsoids are used to exclude any unnecessary checks of ellipsoids. If the outer bounding
 131 spheres of two ellipsoids do not overlap, the two ellipsoids themselves do not overlap
 132 (Figure 2a). If the inner bounding spheres of two ellipsoids overlap, the two ellipsoids
 133 overlap (Figure 2c). Only if the outer bounding spheres overlap and the inner spheres
 134 do not overlap, the overlap check of two ellipsoids is performed (Figure 2b). This simple
 135 method based on bounding outer and inner spheres requires significantly less time than
 136 applying the method in Wang et al. (2001) to all ellipsoids. For combinations of ellipsoids
 137 and line segments, only overlaps between ellipsoids, and ellipsoids and line segments are
 138 checked.

139 Examples of generations of ellipsoids with $d_{a,\max} = 16$ mm, $d_{a,\min} = 8$ mm and $\rho_a = 0.8$,
 140 line segments with $l_f = 30$ mm, $d_f = 0.75$ mm and $\rho_f = 0.01$, and a combination of
 141 ellipsoids and line segments with $d_{a,\max} = 16$ mm, $d_{a,\min} = 8$ mm, $\rho_a = 0.8$, $l_f = 30$ mm,
 142 $d_f = 0.75$ mm and $\rho_f = 0.01$ are shown in Figure 3 for a cell with an edge length of

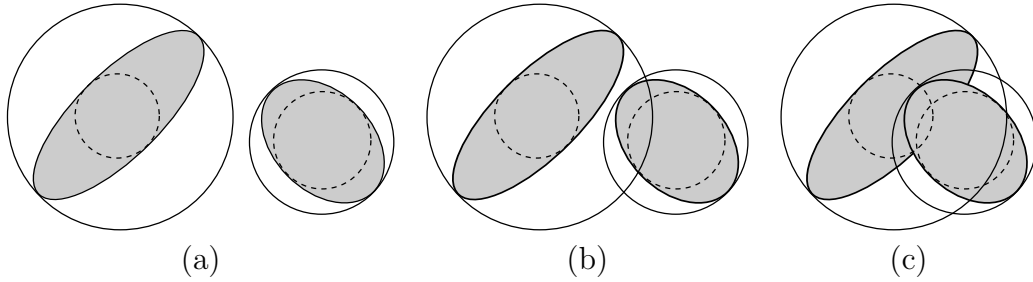


Figure 2: Overlap check of ellipsoids using bounding spheres.

143 100 mm. The fibre diameter d_f is only required to calculate the number of line segments
 144 to be placed, but not for the placement itself. Here, $\rho_a = 0.8$ is the total volume fraction
 145 of ellipsoids, which is significantly greater than the generated volume fraction of 0.23
 146 between the sieve sizes 16 and 8 mm.

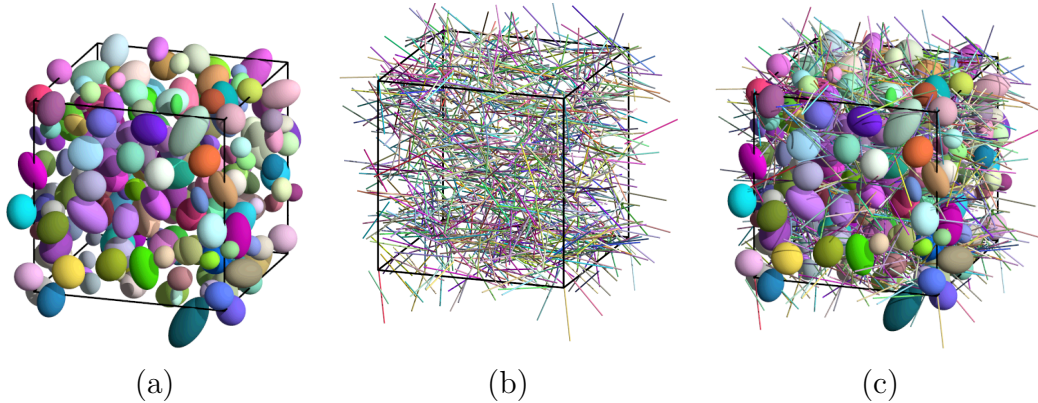


Figure 3: Periodic meso-scale generation for (a) ellipsoids, (b) line segments and (c) combination of ellipsoids and line segments.

147 2.2 Periodic network modelling

148 The fracture processes at the meso-scale are modelled for a periodic cell subjected to
 149 direct tension with a three-dimensional irregular network of discrete structural elements.
 150 The random network generation follows the work in Yip et al. (2005), which was recently
 151 extended to dual structural transport problems in Grassl and Bolander (2016). For the
 152 network generation, random points are placed in the cell using a sequential addition

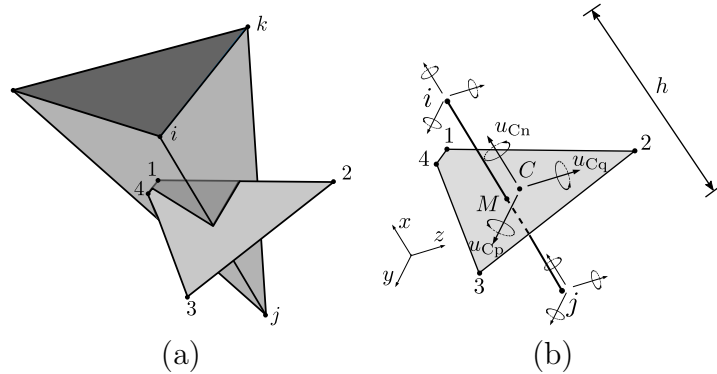


Figure 4: 3D random network: (a) Example of dual Delaunay Voronoi tessellation and (b) structural element with mid-crosssection.

153 approach enforcing a minimum distance d_{\min} between the points (Feder, 1980). These
 154 points are used for dual Delaunay and Voronoi tessellations resulting in randomly arranged
 155 tetrahedra and polyhedra. In Figure 4a, one of these tetrahedra with a common facet of
 156 polyhedra belonging to two vertices of the tetrahedron is shown. The network elements
 157 are placed on the edges of the tetrahedra. The mid-crosssections of the network elements
 158 are set equal to the common facets of the Voronoi cells associated with the element
 159 nodes (Yip et al., 2005). The network elements have six degrees of freedom at each
 160 node which are linked by rigid body kinematics to displacement jumps at the centroid of
 161 the mid-crosssection. These displacement jumps are then related to corresponding stress
 162 components using constitutive models described in Section 2.3.

163 The information of the spatial arrangement of ellipsoids are mapped onto the network.
 164 According to the position of network elements with respect to ellipsoids, network ele-
 165 ments are given the properties of matrix, interfacial transition zone (ITZ) and aggregate.
 166 Network elements with both nodes positioned within an ellipsoid are given stiff elastic
 167 properties representing aggregates. Elements with both nodes located in the matrix are
 168 given properties of mortar with corresponding elastic properties, and strength and frac-
 169 ture energy. Finally, for elements with one node in an ellipsoid and another one in the
 170 matrix or another ellipsoid, the properties of ITZ are used, which are characterised by
 171 lower strength and lower fracture energy than those of the matrix. The stiffness of ITZ

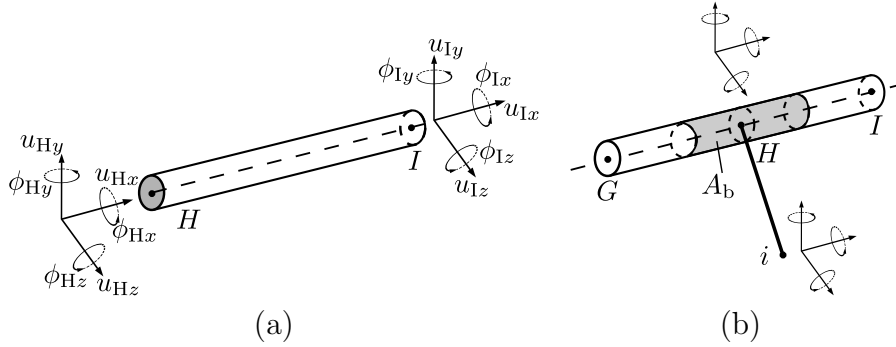


Figure 5: Modelling fibres: a) 3D frame element for fibres and b) link element for the interaction between fibres and matrix.

172 elements are determined by the harmonic mean of the stiffnesses of matrix and aggregate.

173 The fibres are idealised as linear elastic structural frame elements (McGuire et al., 2000),
 174 which are placed on the positions of the line segments (Figure 5a). Interactions between
 175 the frame elements representing fibres and the background network representing matrix
 176 and ITZ are modelled by means of link elements as described in Yip et al. (2005) (Fig-
 177 ure 5b). This type of link elements was originally used for the modelling of bond in
 178 reinforced concrete (Ngo and Scordelis, 1967), and was more recently applied to network
 179 models in Bolander and Saito (1997); Montero-Chac3n et al. (2017). Rigid body kine-
 180 matics are used to determine, from the nodal degrees of freedom of the link and frame
 181 elements, the translation and rotation jumps at the node of the frame element (Figure 5b).
 182 The coordinate system for these jumps is orientated so that one of the axes is aligned
 183 with the axial direction of the frame element. For the translation jump in the direction of
 184 the frame element, an elasto-plastic model described in Section 2.3 is used to model the
 185 slip between the frame element and the background network. For the other components,
 186 a linear force-displacement law with a 1000 times higher stiffness than the elastic stiffness
 187 of the bond law is applied.

188 Reduction of the embedded length due to pullout of the fibres as discussed in detail in
 189 Naaman et al. (1991) is not modelled here, since only small displacements with respect
 190 to the pull-out length are considered. Computationally more efficient semi-discrete ap-

191 proaches described in Kang et al. (2014); Kang and Bolander (2017) would be well suited
 192 to describe the full pull-out process, since these approaches incorporate important features
 193 of the fibre-matrix interaction without modelling individual degrees of freedom.

194 Periodicity with respect to cell boundaries is introduced for both network geometry and
 195 boundary conditions. This is achieved by using a method that was originally proposed
 196 in Grassl and Jirásek (2010) for two-dimensional analyses and then extended to three
 197 dimensions in Athanasiadis et al. (2018) for hydro-mechanical problems. For every random
 198 point placed in the cell, 26 periodic image points in the adjacent cells are created. The
 199 two dual tessellations are then performed for the points in the cell and the periodic image
 200 points. In the resulting network, elements cross the boundaries of the cell. In Figure 6,
 201 the periodic cell with two out of 26 adjacent cells is shown.

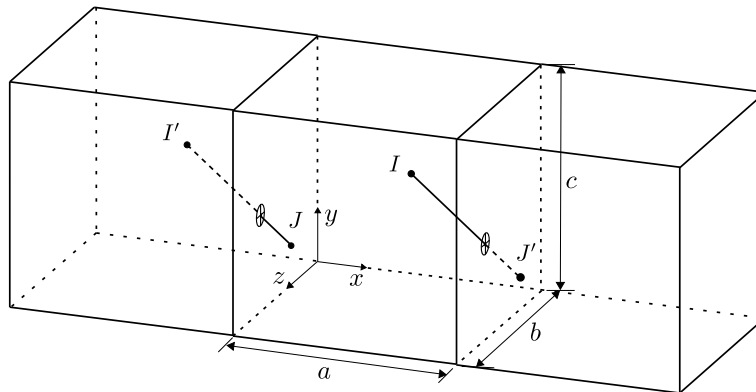


Figure 6: Periodic generation of background network.

202 As an example, elements $I' - J$ and $I - J'$ cross the boundary of the cell. These ele-
 203 ments are used for computing the response of the periodic cell. However, only degrees
 204 of freedom (DOF) of nodes located inside the periodic cell are determined. For nodes
 205 outside the periodic cell (I' and J'), which belong to elements crossing the boundary,
 206 the DOF are determined from those of the periodic image nodes inside the cell (I and
 207 J , respectively) and six average strain components ($\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \varepsilon_{xy}, \varepsilon_{yz}, \varepsilon_{xz}$), which are ap-
 208 plied to the cell. With these average strain components and the work conjugated stress
 209 components ($\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{yz}, \sigma_{xz}$), the loading of the periodic cell is controlled. This
 210 approach has the advantage that localised fracture process zones can occur anywhere in

211 the periodic cell along the direction of loading and are not strongly influenced by the
 212 boundaries of the cell. Analyses of boundary value problems without the use of periodic
 213 boundary conditions would normally require strengthening of the material close to the
 214 ends of the specimen to avoid fracture to occur at the boundaries. Furthermore, in alter-
 215 native formulations of periodic boundary conditions, in which the elements close to the
 216 boundary are aligned so that the nodes are located on the boundary, the periodicity of
 217 the spatial arrangement of the network is not maintained. A detailed description of the
 218 present periodic formulation can be found in Grassl and Jirásek (2010) and Athanasiadis
 219 et al. (2018). This approach is applied to both the background network and the frame
 220 and link elements. An example of the background network representing the three phases
 221 of matrix, aggregates and ITZ is shown in Figure 7a. Fibres with their corresponding link
 222 elements are shown in Figure 7b.

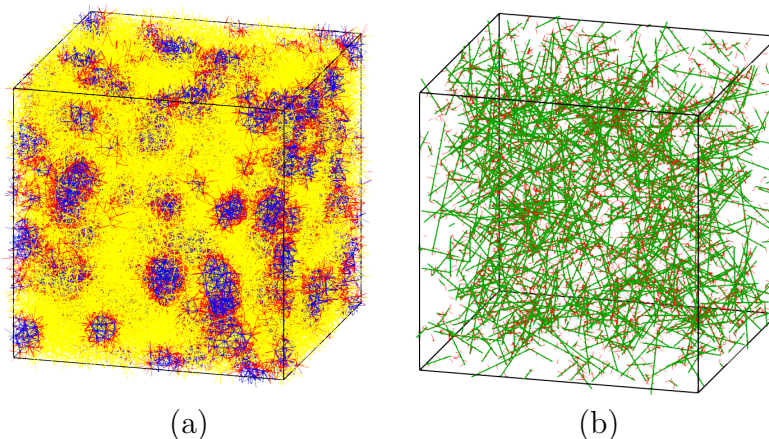


Figure 7: Network model: (a) Network of discrete elements representing matrix (yellow), aggregates (blue) and ITZs (red). (b) Fibre frame elements (green) arranged independently of background network and links (red) connecting fibres to network nodes. Colours refer to online version.

2.3 Constitutive models

224 The constitutive response of the background network representing aggregates, matrix and
 225 ITZs are modelled by linear elasticity and damage mechanics. For matrix and ITZ, a

226 scalar damage model is used of the form

$$\boldsymbol{\sigma} = (1 - \omega) \mathbf{D}_e \boldsymbol{\varepsilon} \quad (4)$$

227 where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are the stress vector and strain vector, respectively, \mathbf{D}_e is the elastic
228 stiffness matrix and ω is the damage parameter ranging from 0 (undamaged) to 1 (fully
229 damaged). For a detailed description of this constitutive model, see Grassl and Bolander
230 (2016).

231 By using the special network generation in Section 2.2 and choosing the stiffness matrix \mathbf{D}_e
232 so that the axial stiffness component is equal to the shear stiffness components, the stress
233 and strain fields are elastically homogeneous and produce zero Poisson's ratio (Yip et al.,
234 2005). A global non-zero Poisson's ratio can be obtained by choosing lower shear than
235 axial stiffness components. However, the elastic response is then no longer homogeneous
236 as discussed in (Yip et al., 2005). This is a shortcoming of the present lattice approach,
237 which can be overcome by techniques described in (Asahina et al., 2017). The influence
238 of the elastic Poisson's ratio on the results of the present analyses is very small, since
239 the response is dominated by nonlinear processes. The onset of damage is determined by
240 an equivalent strain expression which gives an ellipsoidal strength envelope in the stress
241 space with the shear and compressive strength being greater than the tensile strength as
242 described in Grassl and Bolander (2016). The three input parameters for this strength
243 envelope are the tensile strength f_t , shear strength $f_q = 2f_t$ and compressive strength
244 $f_c = 10f_t$. The damage variable is determined from an exponential softening stress-
245 crack opening curve (σ - w_c) with tensile strength f_t and parameter w_f , which controls the
246 slope of the softening curve (Figure 8). The area under the stress-crack opening curve
247 is the fracture energy $G_F = f_t w_f$. With this approach, the resulting load-displacement
248 curves of tensile fracture simulations are independent of the element length, if the inelastic
249 displacements localise in element length dependent zones. The dissipated energy rate \dot{d}

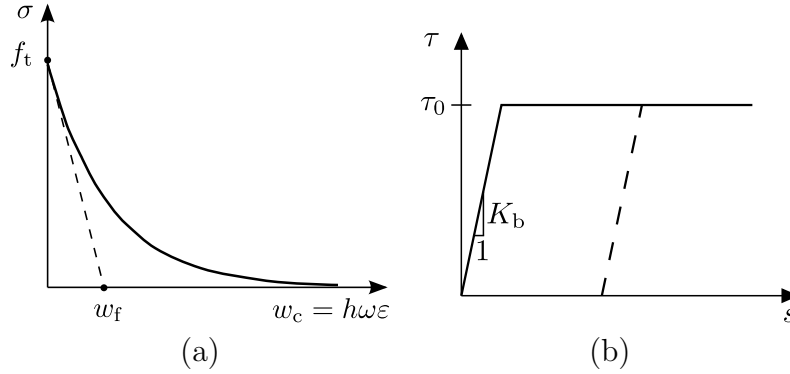


Figure 8: Constitutive models for a) softening in the matrix and b) bond-slip.

250 per unit cross-sectional area in the network element is computed as

$$\dot{d} = h\dot{\omega} \frac{1}{2} \boldsymbol{\varepsilon} : \mathbf{D}_e : \boldsymbol{\varepsilon} \quad (5)$$

251 This dissipated energy is used in Section 4 to present the fracture process zone. Aggregates
 252 are assumed to be elastic. However, fracture in aggregates could be simulated in future
 253 studies with this approach, since aggregates are discretised by multiple network elements.

254 Fibres are modelled to be elastic with a Young's modulus E_s . For the links between the
 255 fibres and the network model, an elasto-plastic model in the tangential direction of the
 256 fibre is used which is illustrated in Figure 8b. Here, τ_0 is the limit stress at which plastic
 257 slip s occurs. The stiffness K_b controls the elastic response of the link. In the analyses, K_b
 258 is set to a large enough value (stated in Section 4) so that the results are not influenced
 259 significantly by it, but small enough so that no numerical problems are created. The
 260 dissipated energy rate \dot{d} per unit area of embedment for the constitutive model of the link
 261 element is

$$\dot{d} = (s - s_p) K_b \dot{s}_p \quad (6)$$

262 Here, \dot{s}_p is the rate of plastic slip.

263 **2.4 Roughness evaluation**

264 The fracture processes are analysed by evaluating the evolution of spatial distribution
 265 of dissipated energy. For the present evaluation, both dissipation due to damage in the
 266 structural network elements, as well as dissipation due to plastic slip in the link elements
 267 are considered. To each element in which energy is dissipated, a crosssectional area with
 268 a centroid as shown in Figure 9 is associated. For the elements used for the background
 269 network, these are the mid-crosssections with the centroid C shown in Figure 4b. For the
 270 link elements, the crosssectional area is A_b shown in Figure 5b and the centroid is the
 271 node of the frame element to which the link element is connected (node H in Figure 5b).

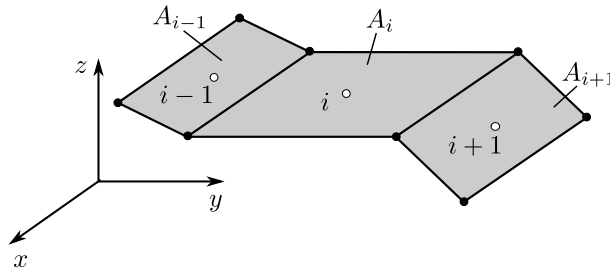


Figure 9: Evaluation of roughness from dissipated energy density of mid crosssections of network elements.

272

273 Firstly, the mean of all heights of centroids of crosssections is calculated as

$$\bar{z} = \sum_{i=1}^N w_i z_i \quad (7)$$

274 Here, z is measured in the direction of the applied tensile strain with the bottom of the
 275 cell used as the origin. Furthermore, w_i are the weights of the individual crosssections,
 276 which are calculated as

$$w_i = \frac{A_i \Delta d_i}{\sum_{k=1}^N A_k \Delta d_k} \quad (8)$$

277 where A_i and Δd_i are the area and increment of dissipation per unit area, respectively,

278 of the facet i . Then, the standard deviation Δh is calculated as

$$\Delta h = \sqrt{\sum_{i=1}^N w_i (z_i - \bar{z})^2} \quad (9)$$

279 This standard deviation is a measure related to the width of the fracture process zone,
280 which takes into account the spatial arrangement and intensity of the dissipation events.
281 It is smaller than the total width of the fracture process zone, which is simply defined
282 as the zone in which energy is dissipated, but does not provide information about the
283 intensity of these events. For a localised crack surface with equal energy dissipation in all
284 elements whose crosssections form this surface, the measure used is equal to the standard
285 deviation of the roughness distribution of the crack surface, which can be determined
286 experimentally as described in Xenos et al. (2015). Because of this geometrical link to
287 the fracture surface, the method is called here roughness evaluation. Nevertheless, for
288 energy dissipation in overlapping zones and fibres, it would not be possible to determine
289 the value of Δh experimentally by means of evaluation of the roughness of the surface
290 alone.

291 **3 Analyses**

292 The network modelling approach described in Section 2 is applied to analyse fracture in
293 cubic periodic cells of an edge length of 100 mm subjected to direct tension as shown in
294 Figure 10. For this setup, the average strain in the axial y -direction (ε_{yy}) is monotonically
295 increased, which results in a reactive stress component in the y -direction (σ_{yy}), which in
296 the presentation of the results is called σ . All other average stress components (σ_{xx} , σ_{zz} ,
297 σ_{xy} , σ_{yz} and σ_{xz}) are kept equal to zero. The analyses are performed quasi-statically with
298 an incremental-iterative approach (see e.g. de Borst et al. (2012)). The iterative part is
299 based on a modified Newton method using the secant stiffness for the damage model for
300 matrix and ITZ, and the elastic stiffness for the elasto-plastic model for the links between

301 fibres and background network.

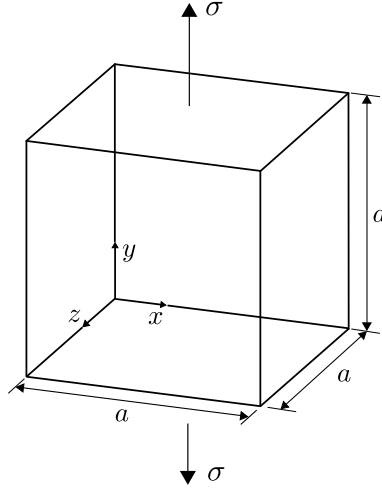


Figure 10: Setup for direct tension analysis with the periodic cell.

302 Four groups of analyses are carried out. For each group, ten random generations of back-
303 ground networks and meso-structures are performed. The network is generated with a
304 minimum distance $d_{\min} = 3$ mm between the randomly placed points. The first group
305 of analyses consists of a network representing matrix without any meso-scale features
306 explicitly incorporated. In the second group of analyses, the network of elements repre-
307 sented matrix, aggregates and ITZs. For these analyses, the volume fraction of aggregates
308 generated with the techniques described in Section 2.1 is $\rho_a = 0.8$ with a maximum and
309 minimum sieve size $d_{a,\max} = 16$ mm and $d_{a,\min} = 8$ mm, respectively. In the third group
310 of analyses, fibres with a length $l_f = 3$ cm, a diameter $d_f = 0.75$ mm and a fibre vol-
311 ume fraction of $\rho_f = 0.01$ are used. Finally, the fourth group consists of combinations
312 of aggregates and fibres with the same input as for the analyses with only one phase.
313 The input parameters for the different phases of the background network are shown in
314 Table 1. These input values are in the typical range of values used for meso-scale analyses
315 of concrete in the literature (Grassl et al., 2012), where it was shown that they provide
316 good agreement with experimental results. For fibres, a modulus of $E_f = 200$ GPa is
317 used. The elastic stiffness and limit stress of the link elements is set to $K_b = 3000$ GPa
318 and $\tau_0 = 4$ MPa, respectively.

Table 1: Input values for the background network. The modulus E of ITZ is determined as harmonic mean of moduli of matrix and particle.

| Phase | E [GPa] | f_t [MPa] | G_F [J/m ²] |
|----------|-----------|-------------|---------------------------|
| Matrix | 30 | 3 | 100 |
| Particle | 90 | - | - |
| ITZ | 45 | 1.5 | 50 |

4 Results

The results of the direct tension analyses of the four groups of material setups are shown in the form of stress-displacement curves, spatial patterns of dissipated energy and roughness-displacement curves. The displacement is determined as the average strain multiplied by the cell length a (Figure 10). For the stress-displacement and roughness-displacement curves, the mean of the quantities of random analyses are shown.

The mean stress-displacement curves for four groups of material setup are shown in Figure 11. For the plain configuration with matrix material only, the stress-displacement curve showed the typical response of quasi-brittle materials subjected to direct tension. In the pre-peak, the response is linear elastic in the first part and then exhibits small non-linearities just before the peak. The post-peak regime shows steep softening, which then flattens with the average stress approaching zero. The peak stress is greater than the input tensile strength, because the stress in the network elements consists of combinations of axial and shear components. With the ellipsoidal strength envelope used, the combined normal and shear stress components result in a greater strength than a pure tensile stress component. The addition of aggregates strongly reduces the peak stress because of the weak ITZs between aggregates and matrix. Furthermore, the initial stiffness is slightly increased due to the greater stiffness of the aggregates. If instead of aggregates only fibres are added to the matrix, the peak stress is only slightly increased compared to the plain peak stress. However, the tail of the stress-displacement curve is strongly influenced by the presence of the fibres with a significant bridging stress present after the initial soft-

340 ening. For combinations of aggregates and fibres, the fibres cause again a small increase
 341 of the peak stress compared to the aggregate only case and result in a similar bridging
 342 stress at the ultimate displacement applied in the analyses.

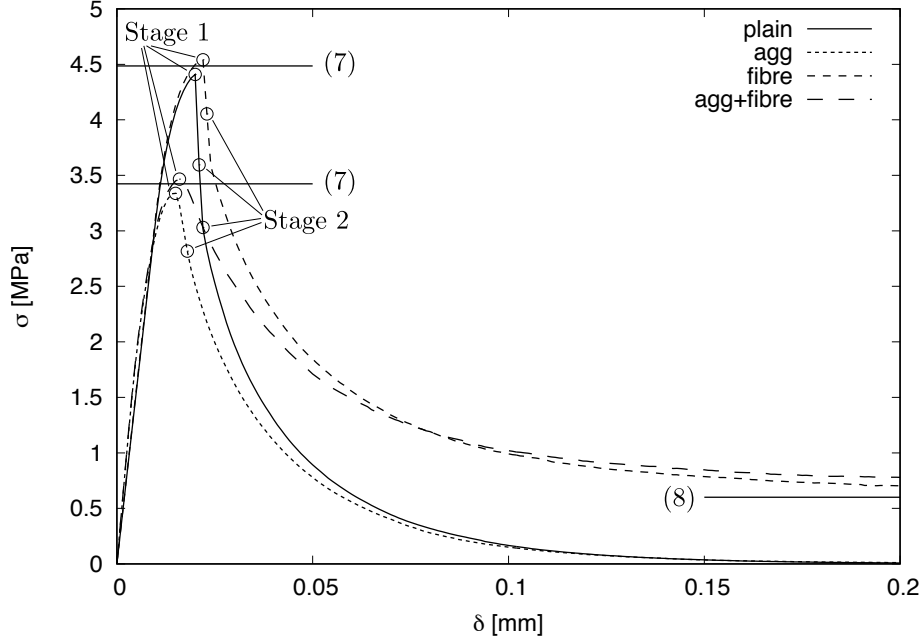


Figure 11: Meso-scale analysis: Mean stress versus displacement for four groups of material setups (plain, aggregates, fibres and aggregates+fibres). The symbols refer to stages for which the crack patterns are shown in Figures 12 and 13. Furthermore, the lines refer to empirical estimates in (10) and (11).

343 For the analyses involving fibres, the peak and bridging stresses are compared to empirical
 344 estimates reported in Naaman (1987). For the peak values of the stress of the analyses
 345 with fibres, the peak stress is

$$\sigma_{cc} = \sigma_{mu} (1 - \rho_f) + \alpha_1 \alpha_2 \tau_0 \rho_f \frac{l_f}{d_f} \quad (10)$$

346 Here, α_1 and α_2 are factors taking into account the fibre orientation and fraction of bond
 347 strength mobilised, respectively. Furthermore, σ_{mu} is the peak stress of the material
 348 without fibres. The stress after cracking is estimated as

$$\sigma_{pc} = 4 \lambda_1 \lambda_2 \tau_0 \rho_f \frac{l_f}{d_f} \quad (11)$$

349 where λ_1 and λ_2 are factors for average pullout length and postcracking orientation effi-
 350 ciency, respectively. These expressions are compared to the numerical results in Figure 11
 351 using $\alpha_1 = 0.5$, $\alpha_2 = 0.2$, $\lambda_1 = 0.25$ and $\lambda_2 = 0.5$, which are typical values for the type
 352 of fibres used. It should be noted that (10) only predicts the increase of strength due to
 353 the presence of fibres, which is very small. The values for σ_{mu} in (10) are obtained for the
 354 corresponding analyses without fibres.

355 All the global stress-displacement curves in Figure 11 exhibit softening which is usually
 356 accompanied by localisation of displacements. Detailed information about the localisation
 357 process is studied in the form of spatial distribution of mid-crosssections at which energy
 358 dissipation occurs. The dissipation patterns for the four groups of analyses are shown in
 359 Figures 12 and 13 for stages at peak and in the post-peak, respectively, for one random
 360 analysis.

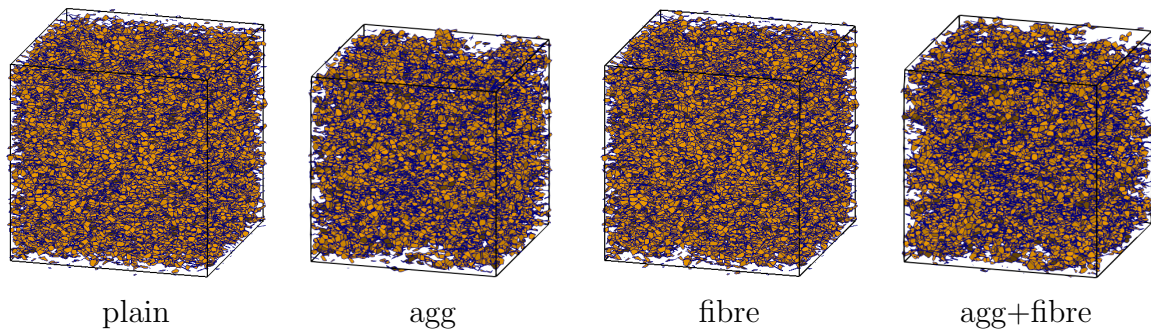


Figure 12: Meso-scale analyses: Crack patterns of direct tension analysis at stage 1 marked in Figure 11. Orange (online version) polygons refer to mid crosssections in which damage increases at this stage of the analysis.

361 The corresponding stages are marked in Figure 11. At stage 1 at peak, the dissipation rate
 362 is distributed in the entire specimen (Figure 12). For plain and fibre analyses, the dissi-
 363 pated energy is distributed uniformly. For analyses involving aggregates, the distribution
 364 is more heterogeneous, because at the position of the elastic aggregates no dissipation
 365 occurs. At stage 2 in the softening regime, the rate of dissipation is strongly localised
 366 (Figure 13). The y-position of the localised region of rate of dissipation differs from the
 367 analysis to analysis because of the periodic cell used. For all groups, the localised zone is

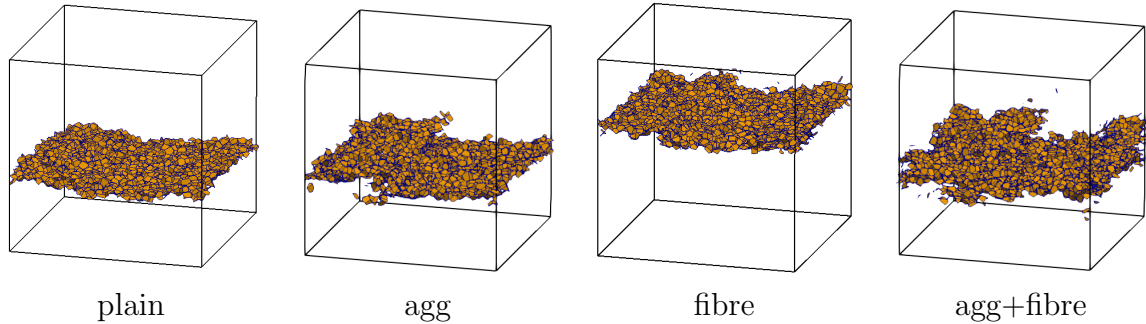


Figure 13: Meso-scale analyses: Crack patterns of direct tension analyses at stage 2 marked in Figure 11. Orange (online version) polygons refer to mid crosssections in which damage increases at this stage of the analysis.

rough. For the plain analyses, this is due to the irregular background network used. For
 368 the other groups, the roughness of the zone of dissipated energy is also influenced by the
 369 heterogeneity in the form of aggregates and fibres. For instance, the spatial distribution
 370 of energy for the aggregate analyses in Figure 13 appears to be wider than for the plain
 371 case. These plots of dissipation rate are from only one random analysis of each group.
 372 Also, all mid-crosssections at which energy is dissipated at this stage of the analysis are
 373 shown without discriminating between the amount of energy that is dissipated at the
 374 crosssections.
 375

For a quantitative representation of the evolution of the zone of rate of dissipated energy,
 376 the roughness measure described in Section 2.4 is used. The mean of the measure of the
 377 width of the fracture process zone Δh in (9) versus displacement is shown in Figure 14.
 378 The symbols in the figure refer to the two stages at which the crack patterns are shown
 379 in Figures 12 and 13. The overall roughness evolutions for the four groups of analyses
 380 are overall very similar. At the start of the analysis, no energy is dissipated, so that
 381 Δh is not defined. For the uniformly distributed cracking in pre-peak regime, Δh is
 382 approximately equal to 30 mm. This value agrees well with the theoretical value for
 383 the standard deviation of a uniform distribution over the cell size, i.e. the interval from
 384 0 to 100 mm, which is $100/\sqrt{12} = 28.9$ mm. At the start of the post-peak regime, the
 385 width of the fracture process zone drops down to values less than 5 mm for all groups
 386

387 of analyses. This drop occurred in the initial part of the softening regime at a stage at
 388 which little energy had been dissipated.

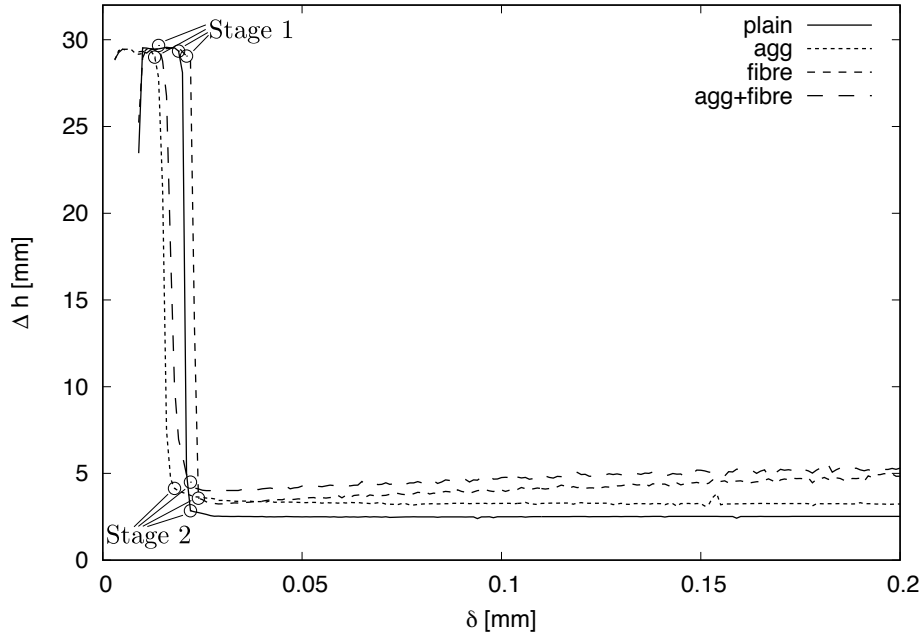


Figure 14: Meso-scale analysis: Measure of width of fracture process zone Δh versus displacement δ for random analyses with aggregates, and with aggregates and fibres. The symbols refer to stages for which the crack patterns are shown in Figures 12 and 13.

389 A detail of the evolution of Δh after the drop is shown in Figure 15. The roughness Δh
 390 is the smallest for the analyses with only the matrix material. After the abrupt drop,
 391 Δh remains almost constant. Adding aggregates results in an increase of the roughness
 392 compared to the plain case. Again, the value remains constant after the drop. If, instead
 393 of aggregates, fibres are added to the background lattice, the roughness is again greater
 394 than for the plain case. However, roughness is not constant with increasing displace-
 395 ment. Instead, it increases with increasing displacement. The same trend is observed if
 396 aggregates and fibres are combined. This increase is due to the energy dissipated by the
 397 slip between fibre and matrix defined in (6). Before the abrupt drop, there is no energy
 398 dissipation due to fibre slip. Only once the crack has formed, the slip between fibres
 399 and matrix starts. In the present approach, fibre pull out is not modelled, which means
 400 that the embedded length of fibres does not change. Consequently, it is expected that
 401 for the analyses involving fibres, Δh would reach a constant value once all fibres crossing

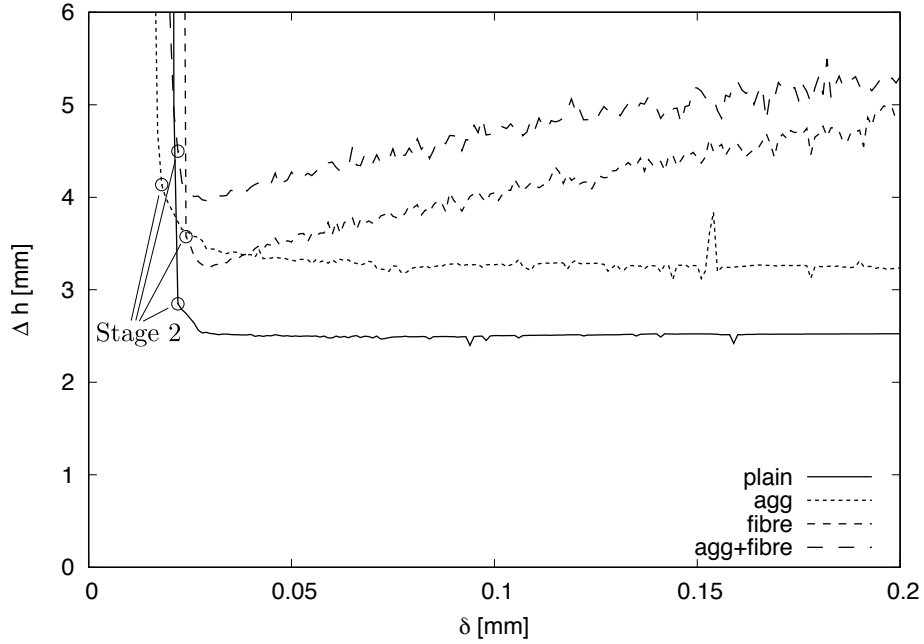


Figure 15: Meso-scale analysis: Stress versus displacement analyses with aggregates and aggregates with fibres. The symbols refer to stages for which the crack patterns are shown in Figures 12 and 13.

402 the localised zone of displacements are significantly stressed so that they dissipate energy
 403 along their short embedded length, and the damage in the matrix so high that the energy
 404 dissipation in the matrix is insignificant. If fibre pullout would be taken into account
 405 as well, the dissipated energy should eventually reduce to zero once all fibres are pulled
 406 out. For a fibre length of 3 cm as used in this study, this point would be reached when
 407 a displacement of 1.5 cm is applied to the specimen, which is 100 times higher than the
 408 maximum displacement considered here.

409 The evolution of dissipated energy for the four groups of analyses is shown in Figure 16.
 410 The symbols refer to the two stages at which the dissipation patterns are shown in Fig-
 411 ures 12 and 13. Here, stage 1 marks the peak of the stress-displacement curves shown
 412 in Figure 11. For all analyses, the dissipation in the pre-peak regime is very small. For
 413 plain and aggregates only cases, the majority of dissipation occurs in the first part of the
 414 post-peak regime and then approaches a constant value. For the analyses with fibres, the
 415 initial dissipation in the very first part of the post-peak regime is slightly less than for

416 the analysis without fibres. However, this difference is very small. In the later stage of
 417 the post-peak regime, the fibres contribute significantly to the dissipation, so that the
 418 overall dissipation of the analyses with fibres is much greater than for aggregates only.
 419 Only fibres, which cross the localised zone shown in Figure 13, are stretched sufficiently
 420 to contribute to the dissipated energy.

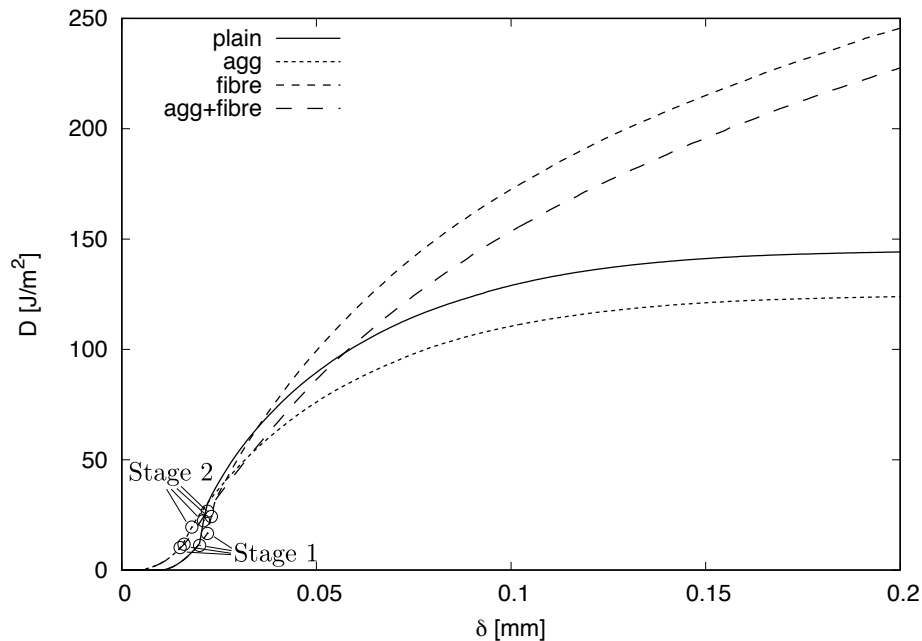


Figure 16: Meso-scale analysis: Dissipated energy D versus displacement δ for the four groups of analyses (plain, aggregates, fibres and aggregates+fibres). The symbols refer to stages for which the crack patterns are shown in Figures 12 and 13.

421 The interplay of energy dissipation in the different phases (matrix, ITZ and slip between
 422 fibres and matrix) is illustrated for the four groups of analyses in Figure 17. From this
 423 figure, it can be seen that fibres only contribute to the dissipation in the post-peak regime
 424 of the stress-displacement curve in Figure 11. Furthermore, the matrix material dissipates
 425 more energy if fibres are present, which is most likely due to the generation of multiaxial
 426 stress states in the material. The dissipation within the ITZs is not affected by the
 427 presence of the fibres, since the majority of energy dissipation in the ITZs occurs early
 428 in the fracture process before the fibres are activated. Furthermore, fibres are placed so
 429 that no overlap with aggregates occurs. Consequently, the ITZs which are located at the
 430 interface between aggregates and matrix would not be expected to be strongly influenced

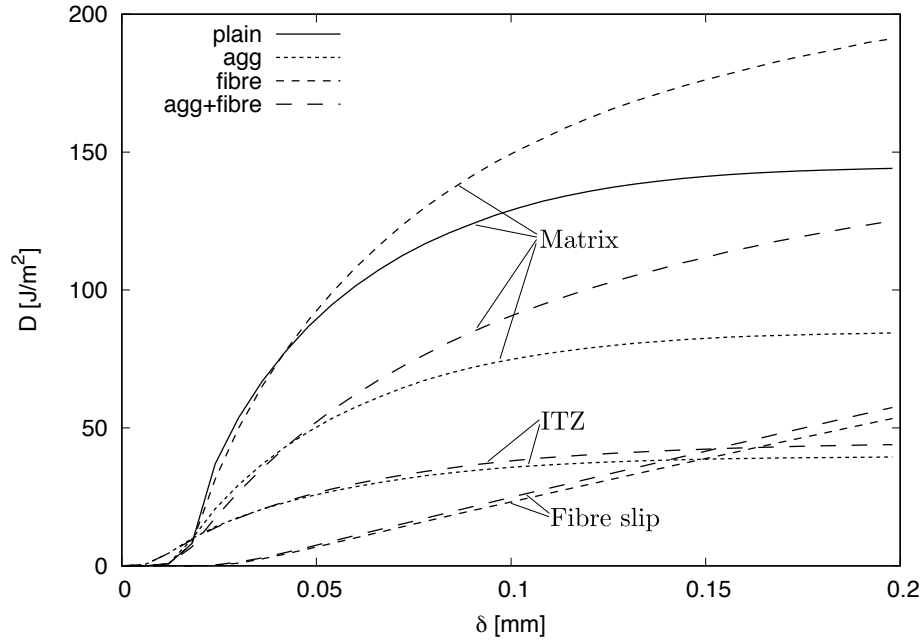


Figure 17: Meso-scale analysis: Dissipated energy D versus displacement δ for the four groups of analyses (plain, aggregates, fibres and aggregates+fibres) in the three phases of material in which energy is dissipated (matrix, ITZ, link be. The symbols refer to stages for which the crack patterns are shown in Figures 12 and 13.

431 by fibres.

432 5 Conclusions

433 Network meso-scale analyses of fracture processes of periodic cells subjected to direct
 434 tension were performed with the aim to investigate the link between material heterogeneity
 435 and width of the fracture process zone. The meso-structures studied here consist of a
 436 quasi-brittle matrix with aggregates, fibres and combinations of aggregates and fibres.
 437 For all material configurations, the width of the fracture process zone reduces abruptly
 438 after the peak load to the width of a rough crack. This strong localisation happens very
 439 early in the post-peak regime at a stage at which very little energy has been dissipated
 440 during the fracture process. For material configurations which include only matrix and
 441 aggregates, the width of the fracture process zone remains constant after the abrupt

442 drop. For material configurations with fibres, the width of the fracture process zone
443 increases after the drop since the slip between fibres and matrix contributes to the energy
444 dissipation.

445 **6 Acknowledgements**

446 The numerical analyses were performed with the nonlinear analyses program OOFEM
447 Patzák (2012) extended by the present authors.

448 **References**

- 449 Asahina, D.; Aoyagi, K.; Kim, K.; Birkholzer, J., and Bolander, J. E. Elastically-
450 homogeneous lattice models of damage in geomaterials. *Computers and Geotechnics*,
451 81:195–206, 2017.
- 452 Athanasiadis, I.; Wheeler, S. J., and Grassl, P. Hydro-mechanical network modelling of
453 particulate composites. *International Journal of Solids and Structures*, 130–131:49–60,
454 2018.
- 455 Barenblatt, G. I. The mathematical theory of equilibrium of cracks in brittle fracture.
456 *Advances in Applied Mechanics*, 7:55–129, 1962.
- 457 Bažant, Z. P. and Jirásek, M. Nonlocal integral formulations of plasticity and damage:
458 Survey of progress. *Journal of Engineering Mechanics, ASCE*, 128(10):1119–1149, 2002.
- 459 Bažant, Z. P. and Oh, B.-H. Crack band theory for fracture of concrete. *Materials and*
460 *Structures*, 16:155–177, 1983.
- 461 Bolander, J. E. and Saito, S. Discrete modeling of short-fiber reinforcement in cementi-
462 tious composites. *Advanced Cement Based Materials*, 6(3-4):76–86, 1997.

463 Bolander, J. E.; Hong, G. S., and Yoshitake, K. Structural concrete analysis using rigid-
464 body-spring networks. *J. Comp. Aided Civil and Infrastructure Engng.*, 15:120–133,
465 2000.

466 Caggiano, A.; Etse, G., and Martinelli, E. Zero-thickness interface model formulation for
467 failure behavior of fiber-reinforced cementitious composites. *Computers & Structures*,
468 98:23–32, 2012.

469 Carol, I.; Prat, P. C., and López, C. M. Normal/shear cracking model: Application to
470 discrete crack analysis. *Journal of Engineering Mechanics*, 123(8):765–773, 1997.

471 de Borst, R.; Crisfield, M.; Remmers, J. J. C., and Verhoosel, C. V. *Nonlinear finite*
472 *element analysis of solids and structures*. John Wiley & Sons, 2012.

473 Dugdale, D. S. Yielding of steel sheets containing slits. *Journal of the Mechanics and*
474 *Physics of Solids*, 8:100–108, 1960.

475 Feder, J. Random sequential adsorption. *Journal of Theoretical Biology*, 87(2):237–254,
476 1980.

477 Grassl, P. and Bolander, J. Three-dimensional network model for coupling of fracture
478 and mass transport in quasi-brittle geomaterials. *Materials*, 9(9):782, 2016.

479 Grassl, P. and Jirásek, M. Meso-scale approach to modelling the fracture process zone of
480 concrete subjected to uniaxial tension. *International Journal of Solids and Structures*,
481 47:957–968, 2010.

482 Grassl, P.; Grégoire, D.; Solano, L. R., and Pijaudier-Cabot, G. Meso-scale modelling of
483 the size effect on the fracture process zone of concrete. *International Journal of Solids*
484 *and Structures*, 49(13):1818–1827, 2012.

485 Grégoire, D.; Rojas-Solano, L. B.; Lefort, V.; Grassl, P.; Saliba, J.; Regoin, J. P.; Loukili,
486 A., and Pijaudier-Cabot, G. Mesoscale analysis of failure in quasi-brittle materials:
487 comparison between lattice model and acoustic emission data. *International Journal of*
488 *Numerical and Analytical methods in Geomechanics*, 2015. DOI: 10.1002/nag.2363.

- 489 Hillerborg, A.; Mod er, M., and Peterson, P. E. Analysis of crack propagation and crack
490 growth in concrete by means of fracture mechanics and finite elements. *Cement and*
491 *Concrete Research*, 6:773–782, 1976.
- 492 Jir sek, M. and Bauer, M. Numerical aspects of the crack band approach. *Computers*
493 *and Structures*, 110–111:60–78, 2012.
- 494 Kabele, P. Multiscale framework for modeling of fracture in high performance fiber re-
495 inforced cementitious composites. *Engineering Fracture Mechanics*, 74(1-2):194–209,
496 2007.
- 497 Kang, J. and Bolander, J. E. Event-based lattice modeling of strain-hardening cementi-
498 tious composites. *International Journal of Fracture*, pages 1–17, 2017.
- 499 Kang, J.; Kim, K.; Lim, Y. M., and Bolander, J. E. Modeling of fiber-reinforced cement
500 composites: Discrete representation of fiber pullout. *International Journal of Solids*
501 *and Structures*, 51(10):1970–1979, 2014.
- 502 Kunieda, M.; Ogura, H.; Ueda, N., and Nakamura, H. Tensile fracture process of strain
503 hardening cementitious composites by means of three-dimensional meso-scale analysis.
504 *Cement and Concrete Composites*, 33(9):956–965, 2011.
- 505 Lange, D. A.; Jennings, H. M., and Shah, S. P. Relationship between fracture surface-
506 roughness and fracture-behavior of cement paste and mortar. *Journal of the American*
507 *Ceramic Society*, 76(3):589–597, 1993.
- 508 Leite, J. P. B.; Slowik, V., and Mihashi, H. Computer simulation of fracture processes of
509 concrete using mesolevel models of lattice structures. *Cement and Concrete Research*,
510 34(6):1025–1033, 2004.
- 511 Leite, J. P. B.; Slowik, V., and Apel, J. Computational model of mesoscopic structure
512 of concrete for simulation of fracture processes. *Computers & Structures*, 85(17):1293–
513 1303, 2007.

514 Li, V. C. and Wu, H. Conditions for pseudo strain-hardening in fibre reinforced brittle
515 matrix. *Applied Mechanics Reviews, ASME*, 74:1134–1141, 2007.

516 McGuire, W.; Gallagher, R. H., and Ziemian, R. D. *Matrix structural analysis*. J. Wiley,
517 New York, 2000.

518 Mehrotra, S. Modelling the aggregate arrangement of concrete. MSc thesis, University of
519 Glasgow, 2011.

520 Mihashi, H. and Nomura, N. Correlation between characteristics of fracture process zone
521 and tension-softening properties of concrete. *Nuclear Engineering and Design*, 165:
522 359–376, 1996.

523 Mihashi, H.; Nomura, N., and Niiseki, S. Influence of aggregate size on fracture process
524 zone of concrete detected with 3-dimensional acoustic-emission technique. *Cement and*
525 *Concrete Research*, 21(5):737–744, 1991.

526 Montero-Chacón, F.; Schlangen, H. E. J. G., and Medina, F. A lattice-particle approach
527 for the simulation of fracture processes in fiber-reinforced high-performance concrete.
528 In *FraMCos-8: Proceedings of the 8th International Conference on Fracture Mechanics*
529 *of Concrete and Concrete Structures*, 2013.

530 Montero-Chacón, F.; Cifuentes, H., and Medina, F. Mesoscale characterization of fracture
531 properties of steel fiber-reinforced concrete using a lattice-particle model. *Materials*,
532 10(2):207, 2017.

533 Morel, S.; Bonamy, D.; Ponson, L., and Bouchaud, E. Transient damage spreading and
534 anomalous scaling in mortar crack surfaces. *Physical Review E*, 78(1):016112, 2008.

535 Mourot, G.; Morel, S.; Bouchaud, E., and Valentin, G. Scaling properties of mortar
536 fracture surfaces. *International Journal of Fracture*, 140(1–4):39–54, 2006.

537 Muller, M. E. A note on a method for generating points uniformly on n-dimensional
538 spheres. *Communications of the ACM*, 2(4):19–20, 1959.

- 539 Naaman, A. E. High performance fibre reinforced cement composites. *IABSE reports*, 55:
540 371–376, 1987.
- 541 Naaman, A. E.; Namur, G. G.; Alwan, J. M., and Najm, H. S. Fiber pullout and bond
542 slip. I: Analytical study. *Journal of Structural Engineering*, 117(9):2769–2790, 1991.
- 543 Ngo, D. and Scordelis, A. C. Finite element analysis of reinforced concrete beams. *ACI*
544 *Journal, Proceedings*, 64:152–163, 1967.
- 545 Otsuka, K. and Date, H. Fracture process zone in concrete tension specimen. *Engineering*
546 *Fracture Mechanics*, 65:111–131, 2000.
- 547 Patzák, B. OOFEM – An object-oriented simulation tool for advanced modeling of ma-
548 terials and structure. *Acta Polytechnica*, 52:59–66, 2012.
- 549 Pijaudier-Cabot, G. and Bažant, Z. P. Nonlocal damage theory. *Journal of Engineering*
550 *Mechanics, ASCE*, 113:1512–1533, 1987.
- 551 Ponson, L.; Bonamy, D.; Auradou, H.; Mourot, G.; Morel, S.; Bouchaud, E.; Guillot,
552 C., and Hulin, J. Anisotropic self-affine properties of experimental fracture surfaces.
553 *International Journal of Fracture*, 140(1-4):27–37, 2006.
- 554 Radtke, F. K. F; Simone, A., and Sluys, L. J. A computational model for failure analysis
555 of fibre reinforced concrete with discrete treatment of fibres. *Engineering Fracture*
556 *Mechanics*, 77(4):597–620, 2010.
- 557 Schauffert, E. A. and Cusatis, G. Lattice discrete particle model for fiber-reinforced
558 concrete. I: Theory. *Journal of Engineering Mechanics*, 138(7):826–833, 2011.
- 559 Schlangen, E. and van Mier, J. G. M. Simple lattice model for numerical simulation of
560 fracture of concrete materials and structures. *Materials and Structures*, 25:534–542,
561 1992a.
- 562 Schlangen, E. and van Mier, J. G. M. Experimental and numerical analysis of the mi-
563 cromechanisms of fracture of cement based composites. *Cement and Concrete Compos-*
564 *ites*, 14:105–118, 1992b.

- 565 Slowik, V. and Leite, J. P. B. Modellierung des mechanischen Verhaltens von Betonen
566 auf der Ebene des Mesogefüges. Technical report, 1999.
- 567 Wang, W.; Wang, J., and Kim, M.-S. An algebraic condition for the separation of two
568 ellipsoids. *Computer aided geometric design*, 18(6):531–539, 2001.
- 569 Xenos, D. and Grassl, P. Modelling the failure of reinforced concrete with nonlocal and
570 crack band approaches using the damage-plasticity model CDPM2. *Finite Elements in*
571 *Analysis and Design*, 117:11–20, 2016.
- 572 Xenos, D.; Grégoire, D.; Morel, S., and Grassl, P. Calibration of nonlocal models for
573 tensile fracture in quasi-brittle heterogeneous materials. *Journal of the Mechanics and*
574 *Physics of Solids*, 82:48–60, 2015.
- 575 Yip, M.; Mohle, J., and Bolander, J. E. Automated Modeling of Three-Dimensional Struc-
576 tural Components Using Irregular Lattices. *Computer-Aided Civil and Infrastructure*
577 *Engineering*, 20(6):393–407, 2005.
- 578 Zhan, Y. and Meschke, G. Multilevel computational model for failure analysis of
579 steel-fiber-reinforced concrete structures. *Journal of Engineering Mechanics*, 142(11):
580 04016090, 2016.