



HAL
open science

Mathematical modelling of uniaxial extension of a heterogeneous gas cell wall in bread dough: Stress fields and stress concentration analysis relating to the proving and baking steps

Kossigan Bernard Dedey, David Grenier, Tiphaine Lucas

► To cite this version:

Kossigan Bernard Dedey, David Grenier, Tiphaine Lucas. Mathematical modelling of uniaxial extension of a heterogeneous gas cell wall in bread dough: Stress fields and stress concentration analysis relating to the proving and baking steps. *Journal of Food Engineering*, 2021, 308, pp.110669. 10.1016/j.jfoodeng.2021.110669 . hal-03279461

HAL Id: hal-03279461

<https://hal.inrae.fr/hal-03279461v1>

Submitted on 13 Jun 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Distributed under a Creative Commons Attribution - NonCommercial 4.0 International License

1 **Mathematical modelling of uniaxial extension of a heterogeneous**
2 **gas cell wall in bread dough: stress fields and stress concentration**
3 **analysis relating to the proving and baking steps**

4

5 **Author names and affiliations**

6 Kossigan Bernard DEDEY ^{1,2}, David GRENIER ^{2*}, Tiphaine LUCAS ²

7 ¹Université Rennes 1, avenue du Général Leclerc, 35042 Rennes Cedex, France

8 ²INRAE, UR OPAALE, F-35044 Rennes, France

9

10

11 kossigan.dedey@inrae.fr, david.grenier@inrae.fr* and tiphaine.lucas@inrae.fr

12

13 ***Corresponding author**

14 INRAE, UR OPAALE, 17 avenue de Cucillé, F-35044 Rennes Cedex, France

15

16 **Abstract**

17 A mathematical model was developed to increase the understanding of stress concentrations
18 within a gas cell wall (GCW) in bread dough during baking. The GCW was composed of a
19 single A-type wheat starch granule surrounded by various proportions of gluten typical of
20 GCWs when about to rupture. Finite element simulations were carried out in 2D using linear
21 viscoelasticity and visco-hyperelasticity. Strain orders of magnitude and rates relevant to
22 dough during baking were applied as boundary conditions for two plausible sets of
23 mechanical properties before and after protein coagulation and starch gelatinization ($T < 50-$
24 60°C and $T > 70-80^{\circ}\text{C}$). The average stress within the GCW was found to be strongly
25 dependent on the starch fraction. Gluten-starch interactions influenced average stress values
26 considerably when the starch fraction was greater than 11% v/v. The locations within the
27 GCW where rupture was most likely to be initiated were identified by mapping maximal
28 stress points using stress field and triaxiality analysis and the findings were discussed.

29 **Keywords: viscoelasticity, visco-hyperelasticity, rupture**

30 **1 Introduction**

31 Bread dough can be viewed as a dispersion of gas cells in a continuous hydrated gluten-starch
32 matrix (Gan et al., 1990). The crumb structure of baked breads (specific volume, gas fraction
33 and texture) mostly depends on dough preparation before baking i.e. mixing and proving
34 (Dobraszczyk, 2017; Eliasson and Larsson, 1993) but also, to a great extent, on the way the
35 walls that separate the gas cells (GCWs) rupture during baking (Dobraszczyk, 2017; Hayman
36 et al., 1998). When early GCW rupture occurs i.e. below both gelatinization and protein
37 coagulation temperatures, the crumb collapses and large cells form within it. When the
38 opposite occurs, and only a few or none of the GCWs rupture during baking, there is
39 shrinkage at the cooling stage that follows due to the decrease in pressure in the cells that
40 have remained closed (Kusunose et al., 1999). At the end of fermentation and during baking,
41 some of the thinnest GCWs are reduced to approximately the size of starch granules
42 (Bloksma, 1990; Sandstedt, 1954). These are the GCWs most likely to rupture. When such a
43 size is reached, gluten and starch granules must be considered as interacting phases to account
44 for their structural heterogeneities. The individual mechanical properties of phases and the
45 interactions between them are crucial to any proper description of stress concentrations and of
46 the areas where rupture is most likely to be initiated within GCWs.

47 The mechanical properties of composite materials such as GCWs in bread dough result from
48 the collective mechanical properties of the separate constituents present in dough and from the
49 interactions between them. In bread dough the chief constituents are starch, gluten and water.
50 Numerous studies have been devoted to the characterization of the individual mechanical
51 properties of gluten (Dreese et al., 1988; Faubion et al., 1985; Janssen et al., 1996; Kokelaar
52 et al., 1996; Ng, 2007; Wesołowska-Trojanowska et al., 2014) and of starch granules
53 (Chiotelli and Le Meste, 2002; Herrera et al., 2017). Studies have been performed at
54 temperatures higher than 25°C on dough or gluten but these are generally carried out using
55 dynamic tests (Dreese et al., 1988). The applied strain and strain rates ($> 10^{-2} \text{ s}^{-1}$) in these
56 studies were greater than those that occur during GCW extension in the course of baking,
57 where strain rates are of the order of 10^{-3} s^{-1} (Lucas et al., 2020). The conditions for most
58 methods are such that the link between rheology and baking performance is not a
59 straightforward one (Dobraszczyk, 2017). During baking, half of the initial extensibility of the
60 gluten is lost at about 65°C and a proportion of the other half by the end of baking (90°C)
61 (Attenburrow et al., 1990; Grenier et al., 2021). In the case of starch alone, studies at
62 temperatures above 25°C have been carried out in excess water (Carrington et al., 1998;

63 Desse et al., 2010; Fisher et al., 1997). At 25°C starch granules are non-deformable at
64 pressures of the order of magnitude found in bread baking. When heated at 65°C in excess
65 water, starch granules soften and become easily deformable (strain > 1.4) under shearing and
66 compression. The behaviour of starch is strongly dependent on water content and the
67 mechanical properties identified in excess water have little or no application to starch at water
68 contents relevant to bread dough during baking. To the best of our knowledge, no work exists
69 that addresses the mechanical properties of starch and gluten separately in controlled
70 hydrothermal conditions relevant to those affecting GCWs during bread dough baking. For
71 this reason, it is hard to obtain the mechanical parameters relevant to the full temperature
72 range encountered during bread dough baking (25-140°C). Only the orders of magnitude of
73 these mechanical properties can be captured. Mohammed et al. (2013) identified values for
74 starch and gluten using Young's moduli of 90 kPa and 10 kPa respectively (with relaxation
75 times of 100 s for starch and 10 s for gluten) for bread dough at room temperature and
76 demonstrated that there was close agreement between numerical simulations and the
77 experimental data. This makes it possible to rely on the orders of magnitude of the moduli
78 selected for the present study.

79 Various constitutive models have been used to describe the mechanical behaviour of dough
80 constituents and compute the stress involved. One mechanical model suited to both gluten and
81 starch during bread dough baking is the "gel" model proposed by Gabriele et al. (2001) and
82 applied by Ng et al. (2006), although others have considered starch to be visco-plastic
83 (Mohammed et al., 2013). A "gel" turns from liquid to solid and makes it possible to mimic
84 phase transitions such as the starch gelatinization and protein denaturation that occur during
85 dough baking. This "gel" material can be modelled using time-dependent models such as the
86 Lodge or Maxwell models using either infinitesimal or finite strain.

87 Views differ on the interactions between starch and gluten. Gluten and starch are known to be
88 chemically incompatible materials and should therefore have limited interactions and should
89 slide along each other (Eliasson and Larsson, 1993). Nevertheless, some authors have
90 reported a number of interactions at the gluten-starch interface in dough (He and Hosney,
91 1992; Mohammed et al., 2013; Petrofsky and Hosney, 1995; Van Vliet et al., 1992), in bread
92 crumb and starch-based biopolymer composites (Guessasma et al., 2015). There is hence no
93 definitive view on the nature of the interactions between gluten and starch in bread dough
94 during baking. To enable the simulation of all possible interactions, Mohammed et al. (2013)
95 used a thin elastic layer that made it possible to simulate either non-cohesive or cohesive

96 interactions at the gluten-starch interface. Such a tool will be likewise be used and further
97 described in this study.

98 There are few works on the numerical modelling of GCW extension at the scale of dough
99 constituents. Mohammed et al. (2013) examined the average stress values in a large number
100 of rheological tests using finite elements and periodic conditions at this scale. It is interesting
101 to note that, unlike the literature and associated modelling for dough rheology, these authors
102 considered dough to be a heterogeneous material composed of gluten, starch and the interface
103 between the two. Unfortunately, stress concentrations and possible locations for rupture
104 initiation in GCWs at strain rates relevant to bread during baking were beyond the scope of
105 their study.

106 Following on from the work carried out by Mohammed et al. (2013), the overall objective in
107 the current study was to extend the microscale approach adopted in dough rheology in terms
108 of the types of law applicable to the mechanical behaviour of dough constituents and the
109 starch fractions, strain-rate range, and variations in the mechanical properties of dough
110 constituents associated with the baking process. Two modelling approaches for the
111 mechanical behaviour of bread dough were compared: linear viscoelasticity (infinitesimal
112 strain) and visco-hyperelasticity (finite strain). This work will subsequently be completed by
113 an analysis of the sensitivity of the computed stress to some of the model's input parameters.
114 In the current study, the process of experimental verification has begun and has been taken as
115 far as possible given the extreme scarcity of input data to feed the model. For this purpose, the
116 average computed stress was compared with the very small amount of experimental data
117 available from the literature for measurements taken at low strain rates on bread dough at
118 ambient temperature. The simulations of the GCW extension were run in two configurations
119 where the starch is stiffer than the gluten and two where the opposite is the case, being
120 representative of the beginning and end of baking, before and after the starch gelatinizes and
121 the proteins denature. The most likely locations for rupture to be initiated within the GCW for
122 these temporally defined configurations, with and without gluten-starch interactions, were
123 analysed through reference to stress fields using the stress triaxiality concept.

124 **2 Materials and methods**

125 **2.1 Geometries**

126 **2.1.1 Estimation of starch fraction in the GCW at the beginning of baking**

127 At the end of proving, the average GCW thickness in wheat dough is 240 μm (Besbes et al.,
128 2013; Turbin-Orger et al., 2012) with an average starch fraction of around 46% v.v
129 (Mohammed et al., 2013). However, the present work focuses on the small proportion of
130 GCWs with a thickness of around 10-15 μm (the average thickness of the largest starch
131 granules) as these are the most likely to rupture (Grenier et al., 2021). To the best of our
132 knowledge very few reports of very thin GCWs in dough are available in the literature, and
133 the present study has processed the microscopic images provided by Sandstedt (1954) that
134 were taken at the end of baking (Fig. 1). The starch fraction was identified by measuring the
135 areas occupied by starch and gluten in the images (Image J, National Institutes of Health,
136 USA). The starch fraction, expressed in m^2 of starch per m^2 of GCW, was found to be 33%
137 for image c in Fig. 1 and may slightly decrease as the GCW becomes thinner, attaining lower
138 values locally where the starch granules are beginning to move apart (see, for example, those
139 shown inside the green box in Fig. 2.a). Very low starch fractions (such as the 8% reference
140 value selected for the present work) are extreme occurrences and are encountered only within
141 strings or strands in bread crumb adjacent to locations where rupture occurs (Stokes and
142 Donald, 2000). The choice of such a low starch fraction for the reference simulation was also
143 intended to facilitate computation at the practical stages of the work and to allow a high strain
144 level to be reached without impeding the location of stress concentrations in the final stages of
145 the work. The fraction was then increased to 11%, 16% and 28% in order to take into account
146 the range of thinner GCWs ready to rupture and to arrive at a closer approximation of the
147 starch fraction reported in the literature in thin GCWs at the end of proving. In the geometries,
148 the starch fraction was increased by adjusting the gluten dimensions (length and width).

149 **2.1.2 Reference simulation**

150 For the reference simulation, the starch fraction was set to 8% v/v because this is the fraction
151 found at the thinnest locations within thin GCWs likely to rupture (Fig. 2.a). Where a GCW is
152 so greatly extended the longest dimension of the starch granule is already aligned within the
153 gluten strip (Bloksma, 1990). The single large and lenticular (A-type) starch granule in cross
154 section measured 10 μm (long half-diameter) by 5 μm (short half-diameter). It was contained
155 within a continuous gluten strip of 100 μm in length (L) and 20 μm wide (l) (Fig. 2.b).

156 2.1.3 Comparison with published experimental results

157 A second 2D geometry was used to compare the computed average stress values with
158 published data at the scale of a continuous dough (section 3.1.3). The geometry was that of a
159 cylinder of dough of 3.75 mm in height and 7.5 mm in diameter and corresponded to that used
160 in Ng et al. (2006) (Fig. 2.c). Axisymmetry was also considered (Fig. 2.d).

161 A third and last 3D geometry (not shown) containing an A-type starch granule ($a = 5 \mu\text{m}$, $b =$
162 $c = 10 \mu\text{m}$) within a gluten strip of 100 μm length, 40 μm width and 20 μm thickness was used
163 only once to check whether the results in 2D were relevant to those in 3D (see section 3.1.1.).

164 2.2 Governing equations

165 2.2.1 Linear viscoelasticity

166 The momentum balance for the quasi-static mechanical equilibrium is given by Eq. 1.

$$167 \nabla \cdot \mathbf{S} = 0 \quad (1)$$

168 The total stress tensor \mathbf{S} is broken down into a purely elastic part and a viscoelastic part as
169 follows (Eq. 2).

$$170 \mathbf{S} = \boldsymbol{\sigma} + \boldsymbol{\tau} \quad (2)$$

171 where $\boldsymbol{\sigma}$ is the tensor (Eq. 3) which describes the time-independent elastic behaviour and $\boldsymbol{\tau}$ the
172 viscoelastic stress tensor which depends on the strain history of the material.

$$173 \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon} \quad (3)$$

174 where \mathbf{C} is the fourth-order tensor of elasticity and $\boldsymbol{\varepsilon}$ is the linear strain tensor (Eq. 4).

$$175 \boldsymbol{\varepsilon} = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \quad (4)$$

176 where \mathbf{u} is the displacement. The viscoelastic stress tensor $\boldsymbol{\tau}$ is derived from the constitutive
177 equation of the 1-element generalized Maxwell equation (Eq. 5).

$$178 \boldsymbol{\tau} + \lambda_r \dot{\boldsymbol{\tau}} = \lambda_r G \dot{\boldsymbol{\gamma}} \quad (5)$$

179 where λ_r is the relaxation time (gluten or starch), $\dot{\boldsymbol{\gamma}}$ is the infinitesimal shear strain rate tensor
180 and G the shear elastic modulus (gluten or starch).

181 2.2.2 Visco-hyperelasticity

182 The momentum balance equation in the case of hyperelasticity is written as Eq. 6.

$$183 \nabla \cdot (\mathbf{FS})^T = 0 \quad (6)$$

184

185 where $\mathbf{F} = \mathbf{I} + \nabla \mathbf{u}$ is the deformation gradient where \mathbf{I} is the second-order unit tensor and \mathbf{u} is
186 the displacement. \mathbf{S} is the second Piola-Kirchoff stress tensor (Eq. 7). It is derived from the
187 strain energy density function (W).

$$188 \mathbf{S} = 2 \frac{\partial W}{\partial \mathbf{C}_c} = \mathbf{S}_{el}^\infty + \mathbf{Q} \quad (7)$$

189 where $\mathbf{C}_c = \mathbf{F}^T \mathbf{F}$ is the right Cauchy-Green deformation tensor (Eq. 8). The elastic stress
190 tensor is given by Eq. 8.

$$191 \mathbf{S}_{el}^\infty = \mathbf{S}_{vol}^\infty + \mathbf{S}_{iso}^\infty = \det(\mathbf{F})^{-1} \mathbf{F}(\mathbf{C} : \boldsymbol{\varepsilon}) \mathbf{F}^T \quad (8)$$

192 where \mathbf{S}_{vol}^∞ and \mathbf{S}_{iso}^∞ are the volumetric and isochoric part, respectively (Holzapfel et al.,
193 2000). The non-linear strain $\boldsymbol{\varepsilon}$ is given by Eq. 9.

$$194 \boldsymbol{\varepsilon} = \frac{1}{2} ((\nabla \mathbf{u})^T + \nabla \mathbf{u} + (\nabla \mathbf{u})^T \cdot \nabla \mathbf{u}) \quad (9)$$

195 The stress in the 1-element viscoelastic generalised Maxwell model is obtained from Eq. 10.

$$196 \mathbf{Q} + \lambda_r \dot{\mathbf{Q}} = \lambda_r \beta \mathbf{S}_{iso}^\infty \quad (10)$$

197 The dimensionless coefficient $\beta > 0$ denotes the strain energy factor and is written as Eq. 11.

$$198 \beta = E_{visco} / E_{el} \quad (11)$$

199 where E_{visco} and E_{el} denote the Young modulus in the viscous branch (time-dependent
200 elasticity) and purely elastic branch (time-independent elasticity) respectively in the 2-branch
201 Maxwell model.

202 In this study, the Neo-Hookean model is used for the strain energy density function (Eq. 12).

$$203 W = \frac{1}{2} \mu (\mathbf{I}_1 - 3) \quad (12)$$

204 where μ is the Lamé coefficient (shear modulus) and $\mathbf{I}_1 = \text{tr}(\mathbf{C})$ is the first invariant of the
205 left Cauchy–Green tensor.

206 **2.3 Initial conditions and boundary conditions**

207 It was assumed that there was initially no stress within either the gluten or the starch.
208 Conclusions on how the stress is concentrated will not be affected, even if that assumption
209 does not stand, provided that discussion is limited to stress increases and to the identification
210 of locations where these are greatest. The comparison to given yield stress cannot, however,
211 be guaranteed.

212 **2.3.1 Reference simulation**

213 Strain rates of the order of 10^1 to 10^2 s^{-1} (Weegels et al., 2003) have been estimated within gas
214 cell membranes during failure in bread dough during proving at $34^\circ C$. These strain rates are
215 relevant to the study of crack propagation and increase in size of a hole within the GCW once
216 a crack has been initiated. In the present study, we only focused on stress concentration before
217 rupture. The extension of the still un-cracked GCW is hence driven by the growth of the gas
218 cells between which it is sandwiched. At the end of proving and during baking, GCWs, before
219 rupture, typically undergo strain rates ranging from 10^{-4} to 5×10^{-3} s^{-1} and Hencky strain
220 above 1 (Dobraszczyk, 2017; Eliasson and Larsson, 1993; Turbin-Orger et al., 2015). The
221 strain rate depends on the GCW location within the loaf and decreases during baking. For the
222 reference simulation, a typical decrease in strain rate at the core of the dough (Lucas et al.,
223 2020) from 3×10^{-3} s^{-1} to 1.15×10^{-3} s^{-1} was used. The displacement $u\left(x, \pm \frac{L}{2}\right)$ was
224 applied accordingly at the upper and lower boundaries (Eq. 13).

$$225 \quad u\left(x, \pm \frac{L}{2}\right) = \frac{L}{2} \dot{\epsilon}(t = 0) t \quad (13)$$

226 where $\dot{\epsilon}(t = 0)$ is the initial strain rate (3×10^{-3} s^{-1}) and t is the current time. The left and
227 right-hand sides of the GCW are free to move (Fig. 2.b).

228 **2.3.2 Comparison with published experimental results**

229 In order to compare the simulations with published experimental results for the cylindrical
230 geometry (Ng et al., 2006), a constant strain rate was applied. Upper and lower boundary
231 displacements were accordingly applied to match the conditions used in the experiment (Eq.
232 14). The right-hand side of the cylinder was free to move and there was no displacement on
233 the axis of symmetry (Fig. 2.d).

$$234 \quad u\left(x, \pm \frac{L}{2}\right) = \frac{L}{2} (e^{\dot{\epsilon}(t=0)t} - 1) \quad (14)$$

235 **2.3.3 The gluten-starch interface: the Thin Elastic Layer (TEL)**

236 Gluten-starch interaction at the gluten-starch interface was modelled using a Thin Elastic
237 Layer (TEL) boundary condition. The thickness of a very thin layer can easily be defined
238 without taking specific areas into account, the thickness e of the water phase at the gluten-
239 starch interface being of the order of hundreds of nanometers at most. The TEL decouples the
240 displacements on the two sides of the boundary. The interface is characterized by the two
241 elastic constants k_n and k_t , in normal (Eq. 15) and tangential (Eq. 16) directions respectively.

$$242 \quad k_n = \frac{E_{\text{int}}(1-\nu_{\text{int}})}{e(1+\nu_{\text{int}})(1-2\nu_{\text{int}})} \quad (15)$$

$$243 \quad k_t = \frac{G_{\text{int}}}{e} \quad (16)$$

244 where ν_{int} is Poisson's ratio, E_{int} is Young's modulus and G_{int} is the shear modulus of the
245 material at the interface. The interaction between gluten and starch was cohesive when E_{int}
246 was set to 10^6 Pa and non-cohesive when it was set to 10^{-6} Pa.

247 **2.4 Material properties**

248 **2.4.1 Reference properties**

249 Both gluten and starch were considered to be viscoelastic. As neither gluten nor starch was
250 assumed to exhibit much time-independent elasticity, the time-independent Young's modulus
251 was set to 10 Pa. Little information on this time-independent elasticity is to be found in the
252 literature, where discussion of the residual stress shown in the experimental data is limited. In
253 the present work, the mechanical behaviours of both gluten and starch were mostly controlled
254 by their time-dependent elasticity as it relaxed. At the beginning of baking, gluten is highly
255 deformable while starch granules are non-deformable at the gas pressure values relevant to
256 baking. As the temperature increases above the range 70-80°C, gluten denaturation and
257 subsequent cross-linking are accompanied by an increase in gluten Young's modulus (Grenier
258 et al., 2021) (Fig. 3). By contrast, the uptake of water by starch granules and the associated
259 phase transitions of starch upon heating are accompanied by a decrease in the rigidity of the
260 starch granules. In excess water, starch granules lose their integrity even under gentle
261 shearing, the temperature at which this transition occurs varying with the starch type.
262 Mechanical testing of individual starch granules immediately after heating in excess water has
263 shown that potato starch granules can become highly deformable at pressures of the order of
264 hundreds of Pa (Carrington et al., 1998; Desse et al., 2010; Fisher et al., 1997). At the levels

265 of hydration relevant to bread dough, the extent of granule softening remains uncertain.
266 Microscopic observations of GCWs revealed that the granules appeared to have flattened
267 significantly in wheat bread crumb (Sandstedt, 1954) and to an extreme extent in bread
268 prepared with low-amylose starch which is reputed to soften/disrupt wheat starch at an earlier
269 point than usual during heating (Kusunose et al., 1999). Where baking occurs at atmospheric
270 pressure, the release of carbon dioxide in gas cells becomes limited in the range of
271 temperatures (above 60-70°C) at which granule softening is likely to occur. This makes it
272 highly improbable that GCWs will reach any great degree of extension in these conditions and
273 there is therefore no sense in studying high levels of extension for such cases. It is relevant to
274 do so, though, for innovative baking processes such as partial vacuum baking (Grenier et al.,
275 2019; Lucas et al., 2016; Rondeau-Mouro et al., 2019; Şimşek, 2020) where extension is
276 forced at mid-baking by the decrease in pressure in the oven's atmosphere. This decrease in
277 pressure is accompanied by water ebullition and gas extension and, consequently, GCW
278 extension is enhanced in these conditions.

279 Two sets of Young's moduli were therefore considered for the computations. The first relates
280 to early baking (before 50-60°C is reached) when the starch (100 kPa) is more rigid than the
281 gluten (10 kPa) (Attenburrow et al., 1990; Dreese et al., 1988; Khatkar and Schofield, 2002;
282 Mohammed et al., 2013), and the second reflects the conditions of advanced baking (beyond
283 70°C) when gluten has low deformability (100 kPa) (Attenburrow et al., 1990) and starch
284 deformability is high (10 kPa) (Fisher et al., 1997) (Fig. 3). The orders of magnitude for the
285 first set derive from the work of Mohammed et al. (2013) and are simply inverted to form the
286 second set because no data for wheat starch at moderate levels of hydration and high
287 temperatures is available in the literature. For the reference simulation, the same relaxation
288 time (10 s) was used for both gluten and starch. These parameters are assumed to remain
289 constant throughout the extension (Fig. 3). All parameters are gathered in Table 1.

290 **2.4.2 Comparison with published experimental results**

291 Since the dough was treated as uniform in the experiment used for validation, the mechanical
292 properties were also considered to be uniform throughout the dough cylinder for that specific
293 case. The average Young's modulus of the dough (100 kPa) was chosen. Two relaxation
294 times (10 and 100 s) were also used in order to evaluate the sensitivity of the average stress to
295 strain rate.

296 **2.5 Digital modelling**

297 Finite element computations were carried out using the COMSOL Multiphysics®
298 v. 5.4 (COMSOL AB, Stockholm, Sweden) MUMPS solver . A mesh convergence test was
299 run to find the best balance between simulation time/use of computer resources and the
300 stability of the model. The average run time varied from 10 minutes to 1 day on an Xeon (R)
301 W-2155 CPU Intel processor at 3.31 GHz, with 256 Go RAM.

302 **2.6 Analysis of stress fields and the triaxiality factor**

303 For stress analysis, the von Mises criterion was applied (Eq. 17). This equivalent tensile stress
304 (known as von Mises stress, σ_{vm}) is that most commonly used for the analysis of yielding in
305 materials science.

$$306 \quad \sigma_{vm} = \sqrt{\frac{(\sigma_{11}-\sigma_{22})^2+(\sigma_{22}+\sigma_{33})^2+(\sigma_{33}+\sigma_{11})^2+6(\sigma_{12}^2+\sigma_{23}^2+\sigma_{31}^2)}{2}} \quad (17)$$

307 The triaxiality factor (*T. F.*, Eq. 18) was also used to identify the regions of uniaxial extension
308 and shear. When the triaxiality factor is around 0.33 the material is mostly uniaxially
309 extended and when it is equal to zero the material is mostly sheared. In the stress, the numbers
310 refer to the direction of the space. The first number is the direction normal to the surface upon
311 which the stress is applied and the second is the direction of the component of the stress.

$$312 \quad T.F. = \frac{\sigma_{eq}}{\sigma_{vm}} \quad (18)$$

313 where $\sigma_{eq} = \frac{1}{3} (\bar{\sigma}) = \frac{1}{3} (\sigma_{11} + \sigma_{22} + \sigma_{33})$

314 **3 Results and discussion**

315 **3.1 Model analysis and experimental validation**

316 Average stress values computed using linear-viscoelasticity in 2D and 3D were compared in
317 order to check that the agreement between them was sufficient for the entire study to be
318 conducted using 2D geometries (section 3.1.1). Viscoelasticity and visco-hyperelasticity
319 approaches were then compared to assess where visco-hyperelasticity was more suited to the
320 task than linear viscoelasticity (section 3.1.2). Last, the average stress values computed using
321 hyperelasticity were compared to previously published experimental data (Ng et al., 2006)
322 (section 3.1.3).

3.1.1 Comparison between 2D and 3D geometries

Fig. 4 shows the average values for von Mises stress vs Hencky strain in 2D and 3D geometries using the reference simulation for the two selected cases (starch granule more rigid than gluten/gluten more rigid than starch granule) (Fig. 4). Where the starch granule was more rigid than the gluten and up to a Hencky strain of 0.67, the difference when using linear visco-elasticity in 2D and 3D did not exceed 2%. Where the gluten was more rigid than the starch granule, this difference reached the order of 20% at most. These discrepancies are in line with those reported by Mohammed et al. (2013). 2D rather than 3D geometry was therefore used to reduce computation times without too greatly distorting the results.

3.1.2 Comparison between linear viscoelasticity and visco-hyperelasticity

The average values for von Mises stress vs Hencky strain up to 0.67 are shown in Fig. 5 for both linear viscoelasticity and visco-hyperelasticity. There was good agreement between simulations up to a strain of 0.08. Thereafter, the average stress values diverged. It is notable in Fig. 5 that, when $E_{\text{starch}}/E_{\text{gluten}}=0.1$, the viscoelasticity model barely registers the strain softening observed experimentally by Ng et al. (2006) at low strain rates. For this reason, we selected the visco-hyperelasticity model for the next steps of the study.

3.1.3 Comparison with published experimental results

The average von Mises stress values computed using the axisymmetric geometry were compared to published experimental results obtained at ambient temperature from dough (Ng et al., 2006). The objective here was solely to validate the structure of the model. It is impossible to achieve greater quantitative validation because the mechanical properties used in the model are unlikely to have been exactly those of the dough used in the experiment. Fig. 6 shows both simulated and experimental average values for stress vs Hencky strain at different strain rates (0.3 s^{-1} and 0.003 s^{-1}). At the high strain rate (0.3 s^{-1}), no good quantitative agreement could be found between the simulations in the present study and the experiments reported in the literature (Fig. 6.a). This is probably due to an overestimate of the Young's modulus. There is unfortunately no guarantee that the elasticity of the dough used by Ng et al. (2006) in their experiment was not lower than that used in the simulation. However, similarities in strain-hardening were observed between the simulation and the experiment performed by Ng et al. (2006) and the stress exhibited almost no sensitivity to relaxation time (Fig. 6.a). Elasticity was the main driver for the stress in this high strain rate configuration. At the low strain rate (0.003 s^{-1}), when the model was less sensitive to elasticity and far more so

355 to viscosity, a quite good quantitative and qualitative agreement was found between the
356 simulations and the experiments (Fig. 6.b). As expected, the average von Mises stress values
357 within the GCW were strongly dependent on the relaxation time at this low strain rate (Fig.
358 6.b). This indicates that the estimation of the relaxation time for dough (or dough
359 constituents) has to be quite accurate when addressing GCW extension during proving or
360 bread baking, since it is the viscous aspect of the dough that mostly drives the stress under
361 such low strain rate conditions. Note that this statement is only true if the assumption of very
362 low time-independent elasticity was true. At low strain rates, precisely the opposite
363 conclusions would be drawn if there were a degree of time-independent elasticity in the
364 dough. In such a case, only time-independent elasticity would be relevant because all possible
365 time-dependent elasticity relaxation would have already occurred.

366 **3.2 Average stress values**

367 **3.2.1 Reference starch fraction**

368 Fig. 7 plots the average values of von Mises stress as a function of the Hencky strain for
369 starch to gluten moduli ratios of 0.1 and 10. The starch-gluten moduli ratios were found to
370 have significant impact on the average von Mises stress. Average stress values where starch
371 was less rigid than gluten were tenfold higher than those where starch was more rigid than
372 gluten. This was largely due to the high proportion of gluten, which accounted for 92% of the
373 total volume.

374 The nature of the interactions between gluten and starch was found to have no effect on the
375 average von Mises stress within the GCW for the reference starch fraction (8%). This does
376 not fit with the reported results of Mohammed et al. (2013), who found that the cohesive/non-
377 cohesive nature of the gluten-starch interface affected average stress values in every case
378 tested in their study. The difference is explained by their choice of starch fraction, which
379 averaged around 46 % in bulk dough without gas cells (Mohammed et al., 2013; Tanner et al.,
380 2011). The following section will address the different starch fractions and will extend the
381 comparison with the data reported by Mohammed et al. (2013).

382 **3.2.2 Effect of starch fraction**

383 Fig. 8 shows the average von Mises stress as a function of Hencky strain for the reference
384 (blue color) starch fractions of 11, 16 and 28% and compares the cohesive and non-cohesive
385 hypotheses concerning the interface between starch and gluten; only the case where the starch

386 is more rigid than the gluten is considered here. The nature of the interaction increasingly
387 affected average von Mises stress values as the starch fraction increased (Fig. 8). From this, it
388 can be concluded that the nature of the gluten-starch interaction affected the average stress
389 within the GCW as soon as the starch fraction exceeded a threshold located between 8% and
390 11%. As expected, the decrease in average stress values that accompanied the increase in
391 starch fraction was greater when the interface was non-cohesive. Slightly greater average
392 stress values were found when a cohesive interface was involved. Indeed, within the area of
393 gluten closest to the starch granule, the increase in starch fraction was accompanied by a
394 greater increase in stress values because the gluten in this area was under greater strain than it
395 was when the interface was non-cohesive.

396 **3.3 Stress fields and triaxiality: stress concentrations in early and late baking**

397 The objective in this section is to refine the foregoing analysis by considering local stresses
398 rather than average values. The intention is to learn more about the most likely locations for
399 GCW rupture in the different configurations. From this point on, we will adopt the working
400 assumption that the locations with the highest concentrations of stress are where the rupture of
401 the material (the GCW in this instance) is most likely to be initiated. In other words, we
402 assume that rupture occurs when the yield stress value is exceeded. In a further step, this
403 analysis will make use of these findings to predict the phenomena most likely to be present in
404 microscopic observations of the GCW in baked bread crumb. It should be remembered that
405 the range of moduli ratios that have been tested in the course of the present work are also of
406 significance to the baking process and to gradual changes in molecular conformation upon
407 heating, as detailed in section 2.4.1.

408 Fig. 9 and Fig. 10 show von Mises stress fields for starch fractions of 8% (reference fraction)
409 and 28% at 0.67 and 0.4 Hencky strains respectively, for different starch-gluten modulus
410 ratios (0.1 and 10) and for cohesive/non-cohesive interactions. We next provide the refined
411 analysis referred to above for the reference fraction. The locations of stress concentrations in
412 the 28% starch fraction were found to be identical to those in the reference fraction. Only the
413 magnitude of stress and strain (0.41) before modelled failure differed.

414

415 3.3.1 Early baking, $E_{\text{starch}} > E_{\text{gluten}}$

416 Fig. 9 a depicts results when the starch granule is more rigid than the gluten for the two
417 gluten-starch interface types: cohesive (left) and non-cohesive (right).

418 Where it was assumed that the interaction at the gluten-starch interface is cohesive, the starch
419 granule reinforced the gluten film and the stress spread through the entirety of the gluten and
420 starch by means of the cohesive interaction (Fig. 9.a, on the left-hand side). The rupture was
421 most probably initiated at two points of extreme stress within the gluten film; one lying a few
422 micrometres away from the starch granule in the direction of the extension within the gluten
423 and another immediately adjacent to the rim of the granule (see arrows in Fig. 9.a, left). The
424 maximum stresses were 1.8×10^3 Pa and 2.08×10^4 Pa for the cohesive and non-cohesive
425 gluten-starch interfaces respectively and were thus separated by an order of magnitude. It is
426 worth remembering that yield stress magnitudes in dough for low strain rates (0.1 s^{-1}) ranged
427 from 0.5 to 1.1×10^3 Pa depending on the quality of the gluten network (Attenburrow et al.,
428 1992; Chin and Campbell, 2005; Dunnewind et al., 2003). Such a thin GCW containing a
429 still-rigid starch particle is likely to have ruptured at a lower Hencky strain than 0.67. This
430 would be all the more probable if a certain amount of stress had been previously stored in the
431 GCW at the beginning of the extension process, as can be expected to occur in proven dough
432 at the beginning of baking.

433 Fig. 9 also shows the triaxiality factor fields that provide information on those areas where
434 unidirectional extension (Fig. 9.c) and shear (Fig. 9.e) occur (cohesive hypothesis shown on
435 left). In those cases where the gluten-starch interface was cohesive, the uniaxial extension
436 within the gluten was strongest close to the rims of the starch granules and spread along the
437 sides of the granules (Fig. 9.c, left). Shear was also found within the gluten in the upper and
438 lower regions close to the gluten-starch interface. This shearing probably increases the
439 likelihood that the interface will rupture at these locations. If the cohesive assumption is valid,
440 these simulations tell us that microscopic observations should reveal gluten in close contact
441 with the starch at the mid-point of the granule's length and gluten shreds near the edges of the
442 granule.

443 By contrast, non-cohesive interactions at the gluten-starch interface caused a concentration of
444 stress that was largely confined to the gluten lying in the direction of the extension close to
445 the very edge of the starch granule (Fig. 9.a, right). This was where the greatest uniaxial
446 extension of the gluten film occurred (Fig. 9.c, right). It was also the point at which the GCW

447 was most likely to rupture. The starch granule did not reinforce the gluten as it had done in the
448 previous case and stress within the granule was much lower (see Fig. 9.b vs 9.a). In this
449 hypothesis, once initiated, rupture will spread within the gluten and is then expected to slide
450 around the starch granule since there is no interaction at the gluten-starch interface. Stress
451 values were also high in the gluten film that was close to the lateral edge of the starch granule
452 (Fig 9.a, right) and this constitutes a second highly plausible location for rupture to occur (see
453 arrow in Fig. 9). If the non-cohesive hypothesis is valid, these simulations tell us that, taking
454 into account the uncertainty as to the degree of slippage, the starch granules located closest to
455 the point of rupture might be partially covered with gluten but, unlike those in the cohesive
456 model, they should be totally free of gluten shreds at their edges.

457 3.3.2 Late baking, $E_{\text{starch}} < E_{\text{gluten}}$

458 Fig. 9.b shows von Mises stress fields at 0.67 Hencky strain when the starch granule was less
459 rigid than the gluten for cohesive (left) and non-cohesive (right) gluten-starch interfaces.
460 When it was sufficiently soft, the starch granule became elongated in the direction of the
461 extension and the stress became concentrated along the lateral surfaces of the starch granule
462 because of the extreme extension of the gluten along both sides of the granule (Fig. 9.b and d,
463 green arrows). The rupture of the gluten was most likely to occur along the surface of the
464 granule where both strain and stress were at their greatest. Here again, with a non-cohesive
465 gluten-starch interface, the surface of the starch granule should be free of gluten following
466 rupture. With a cohesive gluten-starch interface, some gluten should remain on the lateral
467 surfaces of the starch granule. In the direction of extension, the stress decreased with distance
468 from the starch granules. It is possible that the gluten that had previously been strained in these
469 areas when it had been less rigid than the starch (replicating the early stage of baking, see
470 section 3.3.1) had now been attenuated by the elongation of the starch granule and the stress
471 redistributed between the gluten and the starch. Such a change is likely to increase the
472 extensive capacity of the GCW but only if starch granule softening occurs before the gluten
473 has become too stiff. We should note that these two events are not well documented in the
474 literature. Note also that if granule softening were to occur very early in the baking process it
475 is possible that the GCWs might rupture far less frequently, leading to an incomplete opening
476 of the porous structure of the bread's crumb. This would cause the baked dough to shrink
477 during the cooling step. Again, this transition cannot be analyzed further without information
478 on the evolution of the starch modulus during the heating process.

479 This analysis has also revealed that the main difference found between cohesive and non-
480 cohesive interactions at the gluten-starch interface was an element of shear on the side of the
481 granule where cohesive interactions were involved but none where interactions were non-
482 cohesive (Fig. 9.f, left vs right). This explains why the stress spread throughout the starch and
483 gluten and why the maximum stress remained lower than when the gluten-starch interactions
484 were non-cohesive. In this case, the triaxiality factor showed that uniaxial extension and shear
485 mostly decreased with distance from the granule, following the direction of the decrease in
486 stress (Fig. 9.d and f).

487 **3.3.3 About the incompressibility of the starch granule**

488 The conclusions drawn up to this point rely on the hypothesis of incompressibility of the
489 starch granule. Unfortunately we found no literature dealing with Poisson's ratio of starch
490 granule to sustain the hypothesis of incompressibility. In order to identify how far the non
491 validity of the assumption of starch incompressibility could affect the results, simulations
492 were run using Poisson's ratio of 0.3, which is an extreme value for polymers (see
493 supplementary material 1). On the one hand, previous conclusions on the location where the
494 stress concentrates the most were unchanged. On the other hand, the effect of cohesion/non-
495 cohesion between gluten and starch on the mean von Mises stress decreased with decreasing
496 Poisson's ratio. This effect was almost totally cancelled (remaining difference of 2.5%) in the
497 late baking configuration and was quite reduced (-20%) in the early baking configuration,
498 where the starch granule was more rigid than gluten.

499 **Conclusion and future research**

500 Both linear viscoelastic and visco-hyperelastic models were assessed to determine their
501 suitability for the computation of average stress and of stress fields during uniaxial extension
502 within gas cell walls (GCWs) in bread dough during baking. Computation of visco-
503 hyperelasticity involving finite strain was found to be more suited to the task of replicating
504 GCW extension under strain and strain rates close to those encountered during baking. The
505 visco-hyperelasticity model made it possible to describe strain-hardening in sufficient
506 accordance with experimental results (Dobraszczyk; Ng et al., 2006; Van Vliet et al., 1992)
507 for a high strain rate ($\dot{\epsilon} = 3 \cdot 10^{-1} \text{s}^{-1}$). Strain softening was computed at low Hencky strain for
508 a low strain rate ($\dot{\epsilon} = 3 \cdot 10^{-3} \text{s}^{-1}$) in line with the work of Ng et al. (2006). The simulations
509 also demonstrated that proper identification of relaxation times is important for the analysis of

510 low strain rates such as those encountered during baking provided that not too much time-
511 independent elasticity is involved.

512 It was found that the nature of gluten-starch interactions had no significant effect on the
513 average stress for the low starch fraction used as a reference (8%). Whether the gluten-starch
514 interaction was cohesive or non-cohesive did, however, become significant when the starch
515 fraction was increased. For a starch granule fraction of 28%, which was the closest to that
516 reported in the literature for thin GCWs and which was estimated in the present study, the
517 mechanical interaction between starch and gluten was found to have an impact on average
518 stress values, as already evidenced for bulk dough in the literature. The nature of the
519 interactions between starch and gluten during baking is still a matter of debate in the cereal
520 science community. Our simulations confirmed that information on the nature of the
521 interaction at the gluten-starch interface such as that proposed by Jekle et al. (2016) is
522 important for the appropriate modelling of the stress fields within GCWs. The rupture
523 location will depend on the nature of this gluten-starch interaction which can be determined
524 by the presence or absence of a number of gluten shreds along the surfaces of the starch
525 granules located closest to the hole produced by the rupture. This evidence may provide a
526 useful indicator for the future microscopic analysis of holes in the GCWs of bread crumb.
527 This result also confirms that the interaction between starch granules and gluten may affect
528 dough performance and that gluten and starch should be considered in interaction (Gao et al.,
529 2020) rather than separately, as is commonly practiced in the literature. The experimental
530 verification of the model remains insufficient, requiring further experimental work to identify
531 the mechanical properties of dough within the relevant temperature range for baking carried
532 out at low strain rates and in a controlled gaseous environment to reflect real-life conditions
533 for bread dough during baking. Work should first be carried out to estimate the time-
534 independent elasticity of the protein matrix and liquid lamella at the dough-gas interface as
535 this might strongly affect strain-hardening at low strain rates. It is almost impossible to record
536 the low strain rates relevant to dough proving and baking using conventional rheometers. A
537 dedicated experimental device for bubble inflation that is capable of reproducing both low and
538 high strain rates in an atmosphere closely resembling that encountered in gas cells during the
539 baking of real dough must therefore be developed. Such a device would enable the
540 elimination of doubt concerning the mechanical properties of dough at high temperatures and
541 provide data to support the conclusions drawn in the present study. The development of this
542 device will form the next step in our investigation. Second, the possible evolution of the

543 interactions at the gluten-starch interface between the beginning and end of baking and the
544 changes that are even more likely to occur between the end of baking and the end of cooling
545 require analysis. This work is necessary for the appropriate modelling of the stress fields in
546 GCWs during the last stages of bread making to be carried out.

547 **Acknowledgments**

548 The first author, Kossigan Bernard DEDEY, is the holder of a grant from Université Rennes 1
549 and INRAE.

550 **References**

- 551 Attenburrow, G., Barnes, D., Davies, A., Ingman, S., (1990). Rheological properties of wheat
552 gluten. *Journal of Cereal Science* 12(1), 1-14.
- 553 Attenburrow, G.E., Davies, A.P., Goodband, R.M., Ingman, S.J., (1992). The fracture
554 behaviour of starch and gluten in the glassy state. *Journal of Cereal Science* 16(1), 1-12.
- 555 Besbes, E., Jury, V., Monteau, J.-Y., Le Bail, A., (2013). Characterizing the cellular structure of
556 bread crumb and crust as affected by heating rate using X-ray microtomography. *Journal of*
557 *food engineering* 115(3), 415-423.
- 558 Bloksma, A., (1990). Dough structure, dough rheology and baking quality. *Cereals Food*
559 *World* 35(2), 237-244.
- 560 Carrington, S., Fisher, L., Odell, J., (1998). *Microrheology of Swollen Starch Granules, Gums*
561 *and Stabilisers for the Food Industry* 9. Elsevier, pp. 371-380.
- 562 Chin, N.L., Campbell, G.M., (2005). Dough aeration and rheology: Part 2. Effects of flour type,
563 mixing speed and total work input on aeration and rheology of bread dough. *Journal of the*
564 *Science of Food and Agriculture* 85(13), 2194-2202.
- 565 Chiotelli, E., Le Meste, M., (2002). Effect of small and large wheat starch granules on
566 thermomechanical behavior of starch. *Cereal Chemistry* 79(2), 286-293.
- 567 Desse, M., Fraiseau, D., Mitchell, J., Budtova, T., (2010). Individual swollen starch granules
568 under mechanical stress: evidence for deformation and volume loss. *Soft Matter* 6(2), 363-
569 369.
- 570 Dobraszczyk, B., (2017). Dough rheology and breadmaking. Peer review: *Teigrheologie /*
571 *Backeigenschaften Cereal Technology* 01, 4-19.
- 572 Dreese, P., Faubion, J.M., Hosoney, R.C., (1988). Dynamic rheological properties of flour,
573 gluten, and gluten starch doughs. I. Temperature-dependent changes during heating. *Cereal*
574 *Chem.* 65(4), 348-353.
- 575 Dunnewind, B., Sliwinski, E., Grolle, K., Vliet, T.v., (2003). The kieffer dough and gluten
576 extensibility rig-an experimental evaluation. *Journal of Texture Studies* 34(5-6), 537-560.
- 577 Eliasson, A.-C., Larsson, K., (1993). *Cereals in breadmaking: a molecular colloidal approach.*
578 Marcel Dekker, New York (USA).
- 579 Faubion, J., Dreese, P., Diehl, K., (1985). Dynamic rheological testing of wheat flour doughs.
- 580 Fisher, L.R., Carrington, S.P., Odell, J.A., (1997). Deformation mechanics of individual swollen
581 starch granules, in: Frazier, P.J., Donald, A.M., Richmond, P. (Eds.), *Starch: Structure and*
582 *Functionality* Royal Society of Chemistry, pp. 105-114.
- 583 Gabriele, D., de Cindio, B., D'Antona, P., (2001). A weak gel model for foods. *Rheologica Acta*
584 40(2), 120-127.
- 585 Gan, Z., Angold, R.E., Williams, M.R., Ellis, P.R., Vaughan, J.G., Galliard, T., (1990). The
586 microstructure and gas retention of bread dough. *Journal of Cereal Science* 12(1), 15-24.
- 587 Gao, X., Tong, J., Guo, L., Yu, L., Li, S., Yang, B., Wang, L., Liu, Y., Li, F., Guo, J., (2020).
588 Influence of gluten and starch granules interactions on dough mixing properties in wheat
589 (*Triticum aestivum* L.). *Food Hydrocolloids* 106, 105885.
- 590 Grenier, D., Lucas, T., Le Ray, D., (2019). Enhanced aeration of part-baked bread using a
591 novel combination of baking and partial vacuum. *Journal of Food Engineering* 248, 62-70.
- 592 Grenier, D., Rondeau-Mouro, C., Dedey, K.B., Morel, M.-H., Lucas, T., (2021). Gas cell
593 opening in bread dough during baking. *Trends in Food Science & Technology* 109, 482-498.
- 594 Guessasma, S., Bassir, D., Hedjazi, L., (2015). Influence of interphase properties on the
595 effective behaviour of a starch-hemp composite. *Materials & Design* 65, 1053-1063.

596 Hayman, D.A., Sipes, K., Hosene, R., Faubion, J., (1998). Factors controlling gas cell failure in
597 bread dough. *Cereal Chemistry* 75(5), 585-589.

598 He, H., Hosene, R., (1992). Factors controlling gas retention in non-heated doughs. *Cereal*
599 *Chem* 69(1), 1-6.

600 Herrera, M.P., Vasanathan, T., Chen, L., (2017). Rheology of starch nanoparticles as influenced
601 by particle size, concentration and temperature. *Food Hydrocolloids* 66, 237-245.

602 Holzapfel, G.A., Gasser, T.C., Ogden, R.W., (2000). A new constitutive framework for arterial
603 wall mechanics and a comparative study of material models. *Journal of elasticity and the*
604 *physical science of solids* 61(1-3), 1-48.

605 Janssen, A., Van Vliet, T., Vereijken, J., (1996). Rheological behaviour of wheat glutes at
606 small and large deformations. Comparison of two glutes differing in bread making
607 potential. *Journal of Cereal Science* 23(1), 19-31.

608 Jekle, M., Mühlberger, K., Becker, T., (2016). Starch-gluten interactions during gelatinization
609 and its functionality in dough like model systems. *Food Hydrocolloids* 54, 196-201.

610 Khatkar, B.S., Schofield, J.D., (2002). Dynamic rheology of wheat flour dough. II. Assessment
611 of dough strength and bread-making quality. *Journal of the Science of Food and Agriculture*
612 82(8), 823-826.

613 Kokelaar, J.J., van Vliet, T., Prins, A., (1996). Strain hardening properties and extensibility of
614 flour and gluten doughs in relation to breadmaking performance. *Journal of Cereal Science*
615 24(3), 199-214.

616 Kusunose, C., Fujii, T., Matsumoto, H., (1999). Role of starch granules in controlling
617 expansion of dough during baking. *Cereal chemistry* 76(6), 920-924.

618 Lucas, T., Grenier, D., Le Ray, D., (2016). Facility and method for treating food products, such
619 as cellular products, in particular for expanding said products, in: Office, E.P. (Ed.),
620 *EspaceNet*. INRAE, France.

621 Lucas, T., Vanin, F., Ureta, M., Challos, S., Diascorn, Y., Salvadori, V., Grenier, D., (2020).
622 Inflation, squeezing and collapse in wheat flour dough during baking: Effects of flour quality
623 and oven temperature. *Journal of Cereal Science* 95, 103017.

624 Mohammed, M.A.P., Tarleton, E., Charalambides, M.N., Williams, J., (2013). Mechanical
625 characterization and micromechanical modeling of bread dough. *Journal of Rheology* 57(1),
626 249-272.

627 Ng, T.S., (2007). Linear to nonlinear rheology of bread dough and its constituents.
628 Massachusetts Institute of Technology.

629 Ng, T.S., McKinley, G.H., Padmanabhan, M., (2006). Linear to non-linear rheology of wheat
630 flour dough. *Applied Rheology* 16(5), 265-274.

631 Petrofsky, K., Hosene, R., (1995). Rheological properties of dough made with starch and
632 gluten from several cereal sources. *Cereal Chemistry* 72(1), 53-57.

633 Rondeau-Mouro, C., Godfrin, C., Cambert, M., Rouillac, J., Diascorn, Y., Lucas, T., Grenier, D.,
634 (2019). Characterization of gluten-free bread crumb baked at atmospheric and reduced
635 pressures using TD-NMR. *Magnetic Resonance in Chemistry* 57(9), 649-660.

636 Sandstedt, R., (1954). The microscopic structure of bread and dough. *Cereal Chem.* 31, 43-
637 49.

638 Şimşek, S.T., (2020). Evaluation of partial-vacuum baking for gluten-free bread: Effects on
639 quality attributes and storage properties. *Journal of Cereal Science* 91, 102891.

640 Stokes, D., Donald, A., (2000). In situ mechanical testing of dry and hydrated breadcrumb in
641 the environmental scanning electron microscope (ESEM). *Journal of Materials Science* 35(3),
642 599-607.

643 Tanner, R.I., Qi, F., Dai, S., (2011). Bread dough rheology: an improved damage function
644 model. *Rheologica acta* 50(1), 75-86.

645 Turbin-Orger, A., Babin, P., Boller, E., Chaunier, L., Chiron, H., Della Valle, G., Dendievel, R.,
646 Réguerre, A., Salvo, L., (2015). Growth and setting of gas bubbles in a viscoelastic matrix
647 imaged by X-ray microtomography: the evolution of cellular structures in fermenting wheat
648 flour dough. *Soft matter* 11(17), 3373-3384.

649 Turbin-Orger, A., Boller, E., Chaunier, L., Chiron, H., Della Valle, G., Réguerre, A.-L., (2012).
650 Kinetics of bubble growth in wheat flour dough during proofing studied by computed X-ray
651 micro-tomography. *Journal of Cereal Science* 56(3), 676-683.

652 Van Vliet, T., Janssen, A.M., Bloksma, A.H., Walstra, P., (1992). Strain hardening of dough as
653 a requirement for gas retention. *Journal of Texture Studies* 23(4), 439-460.

654 Weegels, P.L., Groeneweg, F., Esselink, E., Smit, R., Brown, R., Ferdinando, D., (2003). Large
655 and fast deformations crucial for the rheology of proofing dough. *Cereal Chem* 80(4), 424-
656 426.

657 Wesółowska-Trojanowska, M., Tomczynska-Mleko, M., Mazurkiewicz, J., Kwiatkowski, C.,
658 Kowalczyk, K., Sołowiej, B., Mleko, S., (2014). Rheological properties of gluten obtained from
659 polish wheat cultivars. *Bulgarian Journal of Agricultural Science* 20(5), 1221-1226.

660

661

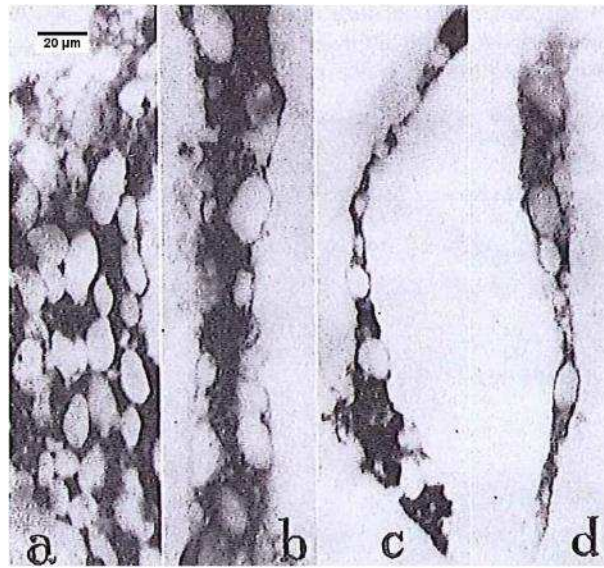


Fig. 1. Microscopic views of GCW cross-sections at the end of fermentation from Sandstedt (1954): a. thick GCW; b., c. and d. thin GCWs.

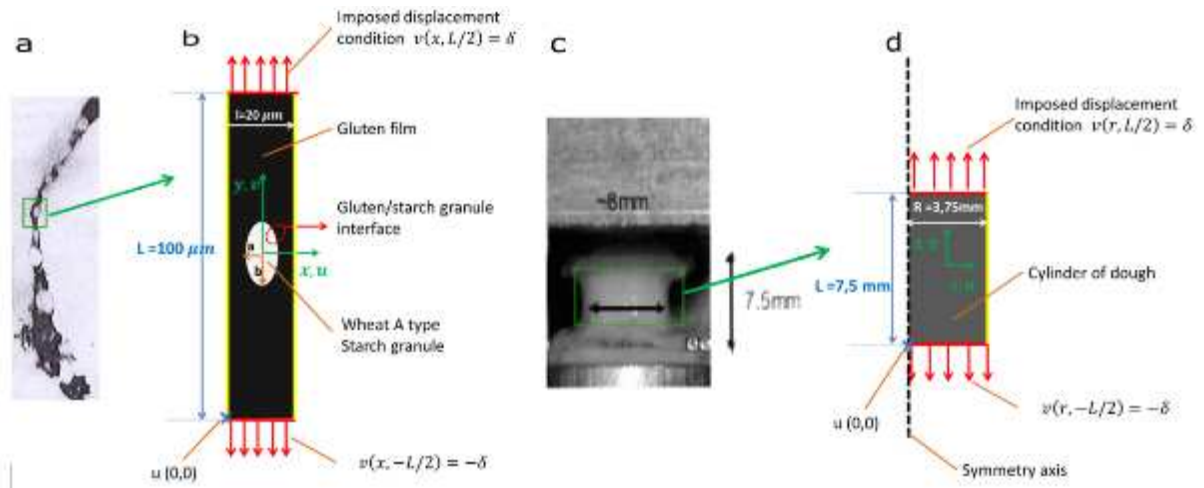


Fig. 2. Geometries and boundary conditions: a. cross-section of a gas cell wall (GCW) about to rupture at the end of proving (Sandstedt, 1954); b. 2D reference geometry for simulations; c. cylindrical geometry of filament stretching experiments in Ng et al. (2006); d. 2D axisymmetric model-validation geometry based on the filament stretching experiment shown in c.

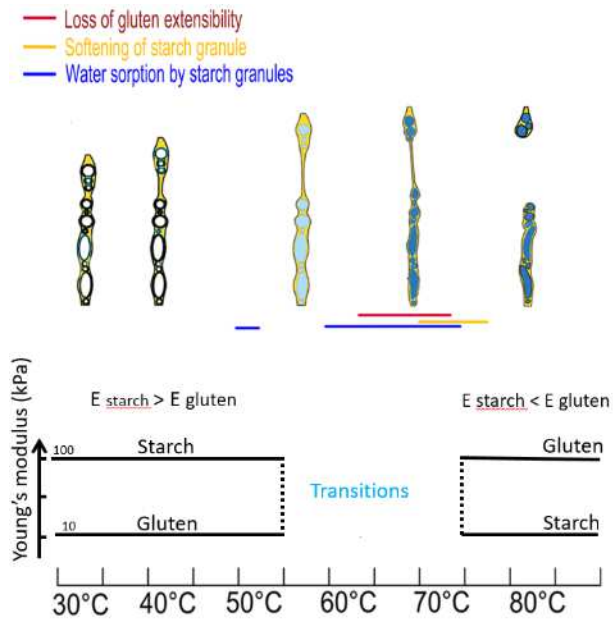


Fig. 3. Mechanical properties for $T < 50-60^{\circ}\text{C}$, $E_{starch}/E_{gluten}=10$ (early in baking) and $T > 70-80^{\circ}\text{C}$, $E_{starch}/E_{gluten}= 0.1$ (later in baking). The GCW spatial organisation and morphology shown in the upper part of the figure has been adapted from Grenier et al. (2021).

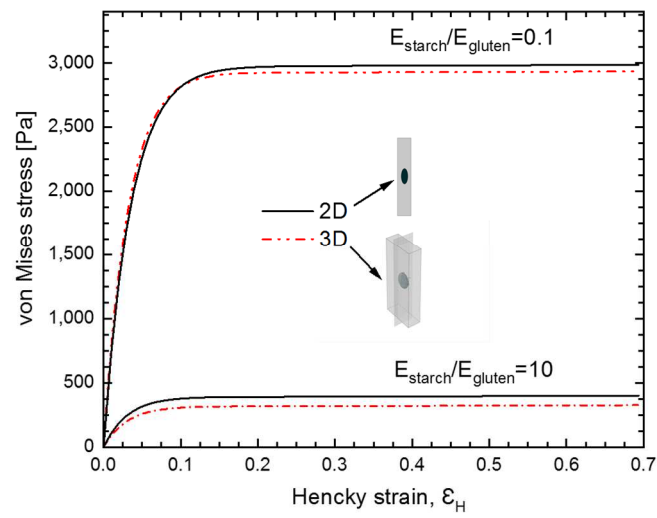


Fig. 4. Average values for von Mises stress vs Hencky strain in the case of **cohesive** interaction at the gluten-starch interface.

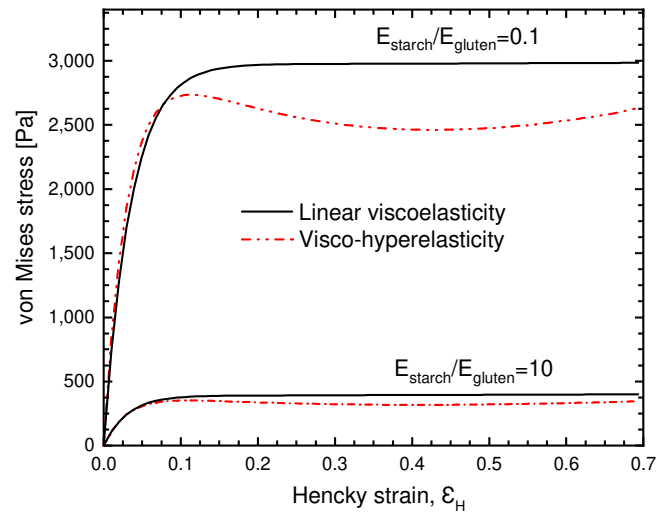


Fig. 5. Plotted average values for von Mises stress vs Hencky strain, comparing linear viscoelasticity with visco-hyperelasticity where there is cohesive interaction at the gluten-starch interface.

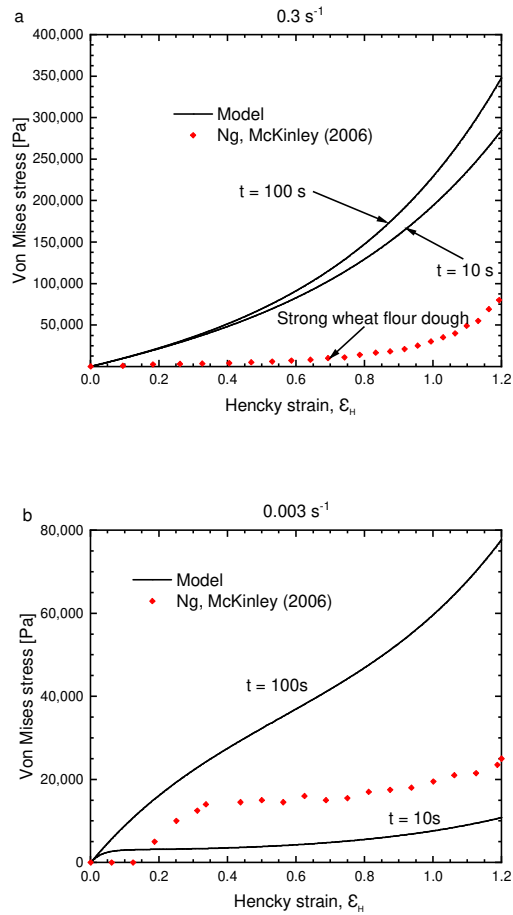


Fig. 6. Average values for von Mises stress vs. Hencky strain, comparing the proposed model with experimental data obtained at two different strain rates (0.3 s^{-1} and 0.003 s^{-1}) (Ng et al., 2006).

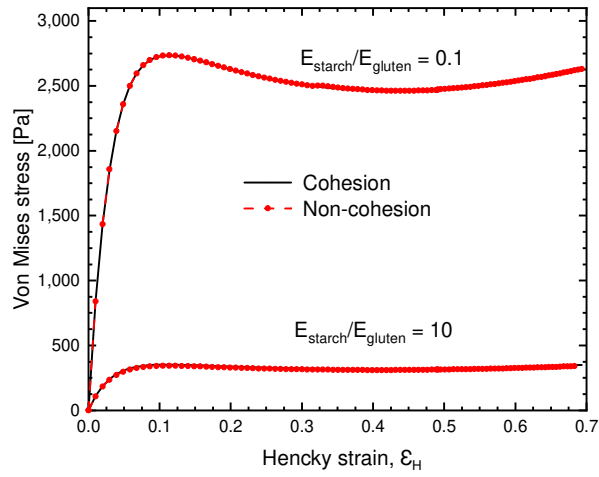


Fig. 7. Reference starch fraction – average values for von Mises stress vs Hencky strain computed with the proposed model for both the cohesive and non-cohesive gluten-starch interface hypotheses and for two different starch-gluten modulus ratios $E_{\text{starch}}/E_{\text{gluten}} = 0.1$ and $E_{\text{starch}}/E_{\text{gluten}} = 10$.

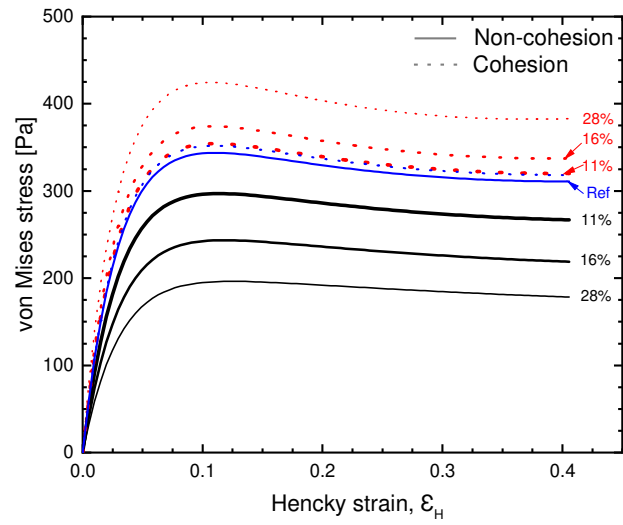


Fig. 8. Starch fractions – average values for von Mises stress vs Hencky strain computed with the proposed model, for different starch fractions (11%, 16% and 28%), the last being of relevance to GCWs in bread dough at the end of fermentation. All calculations were performed for the case $E_{\text{starch}}/E_{\text{gluten}} = 10$.

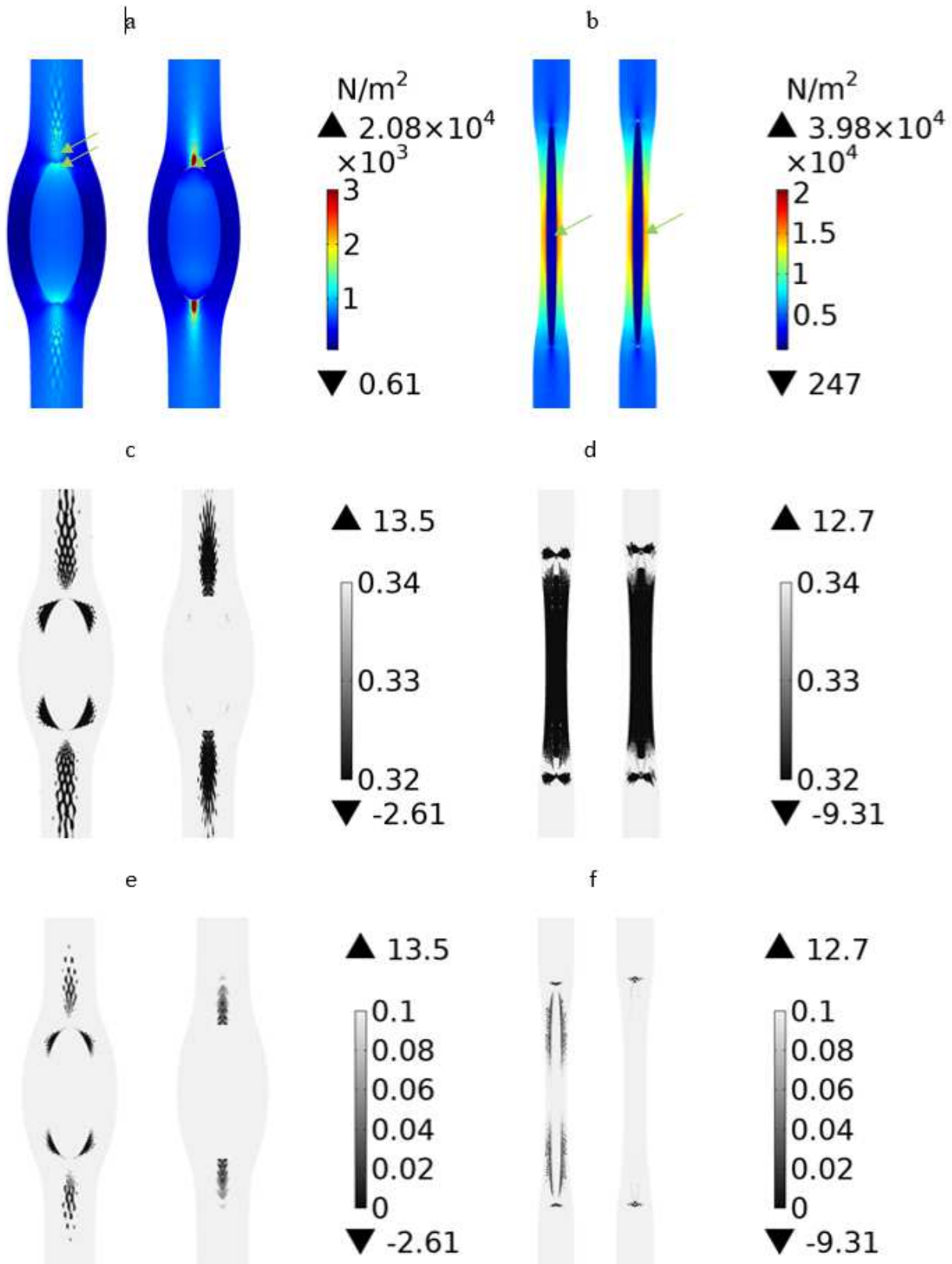


Fig. 9. von Mises stress fields within the GCW at the end of extension (0.67 Hencky Strain) for the two references $E_{\text{starch}}/E_{\text{gluten}}=10$ (a, c, e) and $E_{\text{starch}}/E_{\text{gluten}} = 0.1$ (b, d, f). Triaxiality factor: uniaxial extension (TF = 0.33, c and d) and shear (TF = 0, e and f). Cohesive (left-hand image) and non-cohesive (right-hand image) gluten-starch interfaces are shown for each subplot a, b, c, d, e and f.

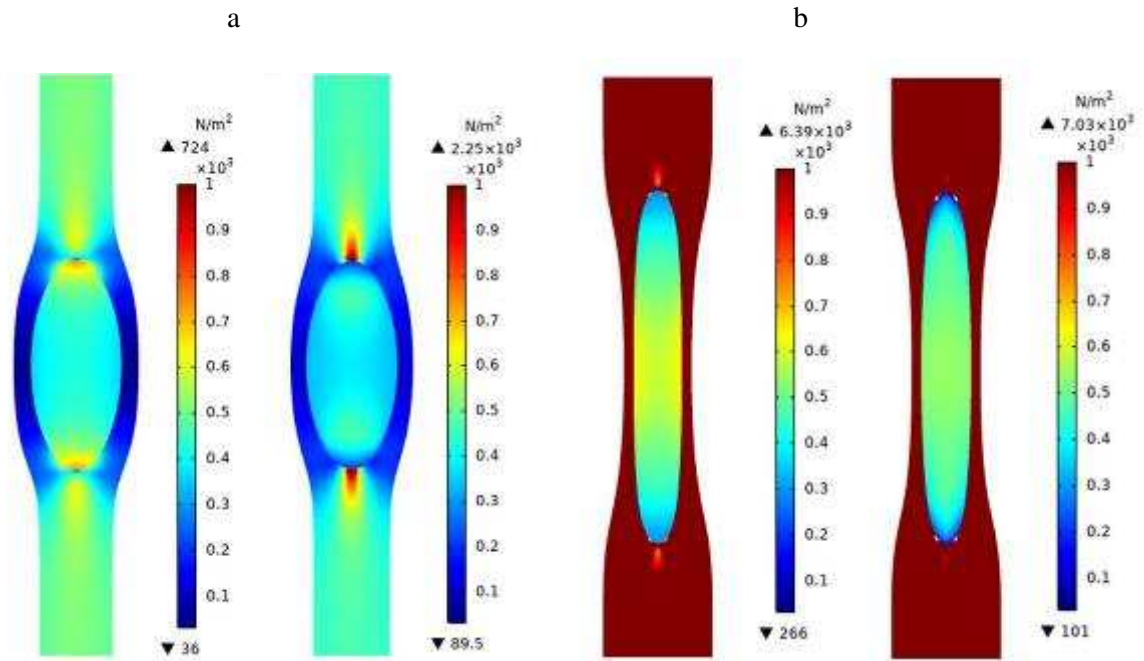


Fig. 10. von Mises stress fields within the GCW at the end of extension (0.41 Hencky Strain) for a 28% starch fraction where $E_{\text{starch}} > E_{\text{gluten}}$ (a) and $E_{\text{starch}} < E_{\text{gluten}}$ (b). Cohesive (left-hand image) and non-cohesive (right-hand image) gluten-starch interfaces are shown for each subplot.

Table 1. Nomenclature and input parameters

		Unit	Value	Ref
Letters				
a	Half of the smallest dimension of the starch granule (A-type)	m	10×10^{-6}	[6]
b, c	Half of the largest dimension of the starch granule (A-type)	m	5×10^{-6}	
C	Fourth-order tensor of elasticity			
C_c	Right Cauchy-Green deformation tensor			
e	Thickness of the material at the gluten-starch interface	m	1×10^{-6}	
E	Time-independent elasticity	Pa	10	
E _{gluten}	Young's modulus of gluten	kPa	T < 50-60°C : 10 T > 70-80°C: 100	[21]
E _{starch}	Young's modulus of starch		T < 50-60°C: 100 T > 70-80°C: 10	
E _{int}	Young's modulus at the gluten-starch interface	kPa	Cohesion: 10^6 Non-cohesion : 10^{-6}	
F	Deformation gradient			
G _i	Shear elastic modulus of material i	Pa	$\frac{E_i}{2(1 + \nu_i)}$	
I	Second-order unit tensor			
I₁	First invariant of the left Cauchy-Green tensor			
k	Elasticity constant of the material at the interface	N/m ³		
l	Smallest dimension of the gluten strip	m	20×10^{-6}	
L	Largest dimension of the gluten strip or height of the cylinder	m	100×10^{-6}	
Q	Stress in the 1-element viscoelastic generalised Maxwell			
r	Horizontal direction axisymmetric			
S	Total stress tensor			
t	Time	s		
u	Displacement vector which components are u in the directions x or r and v in direction y or z	m		
W	Strain energy density function			
x	Horizontal direction			
y	Vertical direction			
z	Vertical direction axisymmetric			
Greek letters				
β _{gluten}	Strain energy factor of gluten		T < 50-60°C: 100 T > 70-80°C: 1000	
β _{starch}	Strain energy factor of starch		T < 50-60°C: 1000 T > 70-80°C: 100	
ε	Linear or Cauchy strain tensor			
ε _H	Hencky strain		$\epsilon_H = \ln(1 + \epsilon)$	
ε̇	Strain rate	s ⁻¹		
μ	Lamé coefficient (shear modulus)			
ν _{int}	Poisson's ratio		Cohesion: 0.4999 Non-cohesion : 0.4999999999 ~ 0.4999	
ν _i	Poisson's ratio of material i			
σ	Time-independent stress tensor	Pa		
σ	Stress	Pa		
τ	Viscoelastic stress tensor	Pa		
γ	Infinitesimal shear strain tensor			
γ̇	Shear strain rate	s ⁻¹		
λ _r	Relaxation time	s		
Super and sub -script				
el	Elastic			
eq	Equivalent			
int	Interface			
Iso	Isochoric			
n	Normal direction			
t	Tangential direction			
T	Transpose			
vm	Von Mises			
vol	Volumetric			
∞	Infinity symbol			