Numerical Simulation of Stress Distribution in Heterogeneous Solids during High Pressure Processing

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Abstract

22 It is generally assumed that the internal stress distribution in foods under high
23 pressure processing (HPP) is uniform, which may not be true for solid foods with
24 hard inclusions, like meats with bones or for particulate foods. Our objective was
25 to simulate the internal stress distribution during HPP of a model heterogeneous
26 solid food made with a gel and a wood inclusion and determine how mechanical
27 properties affect the internal stress distribution. It was determined that hydrostatic
28 pressure decreased and shear stress was generated at the interface between the soft
29 solid and the hard inclusion. The differences in pressure and shear stresses
30 increased as the shear modulus of the soft solid increased. Our studies suggest that
31 a better understanding of the mechanical properties that affect the development of
32 the internal stress field is needed, since they could affect the achieved microbial
33 inactivation levels at different locations in HPP solid foods.

34 **1. Introduction**

35 The increasing demand for natural and less processed foods has triggered
36 novel approaches to food preservation that aim at substituting thermal processing
37 and the use of chemical preservatives with non-thermal processes that can extend
38 the shelf life and improve microbial safety of high value-added products. In the
39 last few years, high pressure processing (HPP) has gained acceptance because it
40 can significantly reduce the microbial load without triggering extensive changes
41 in the physical-chemical attributes of food products. Despite having a high initial
42 capital investment, HPP technology can address the demands of consumers who
43 prefer foods without preservatives while retaining most of the sensorial
44 characteristic of freshness. Furthermore, since the pressure treatment is not
45 dependent on size, shape or mass, unlike thermal treatments, the processing time
46 can be greatly reduced for irregularly shaped large samples.

47
48 HPP of food products was firstly reported by **Hite (1889)**, who was able to
49 extend the shelf life of milk. Major HPP research programs were established in
50 United States, Europe, and Japan in the late 1900s and they demonstrated that
51 HPP is a useful technology in extending the shelf life of foods. Today HPP is a
52 well-accepted technology in Europe and United States for products such as sliced
53 ham, oysters, clams, guacamole, fruit juices, fruit purees, ready-to-eat meals, dips,
54 salsas, etc. (**Avure Technologies, 2014; Hiperbaric, 2014**). Products treated by

55 HPP do not need a specific label in the United States (**Garriga and Aymerich,**
56 **2009**). A high acceptability (67%) of HPP products by consumers was reported
57 for France, Germany, and United Kingdom (**Baron et al., 1999**). It has been
58 shown that HPP is applicable to microbial inactivation in meat products at many
59 stages of processing (**Gola et al., 2000; Yuste et al., 2000**). Numerous reviews
60 have been published on the effects of HPP on microbial inactivation and chemical
61 reactions in food products (**Rastogi et al., 2007; Norton and Sun, 2008;**
62 **Campus, 2010; Rendules et al., 2011; Martinez-Monteagudo and Saldaña,**
63 **2014**).

64
65 One of the main advantages of HPP over thermal pasteurization, from the
66 processing point of view, is that the pressure is considered or assumed to be
67 transmitted uniformly and quasi-instantaneously throughout the sample,
68 regardless of size, shape or packaging (**Barbosa-Cánovas et al., 2005; Sun,**
69 **2005; Brennan, 2006; Doona and Feeherry, 2007; Rastogi et al., 2007;**
70 **Rendueles et al., 2011**). While this is clearly true for liquids and homogeneous
71 solids, the published literature generally reports that there are no limitations to the
72 validity of uniform pressure distribution. The only dissenting work is by
73 **Minerich and Labuza (2003)** who did not offer any mechanistic explanation for
74 their findings. They determined that the pressure at the center of a piece of ham
75 during HPP was significantly lower, by 9 MPa, than the applied external

76 hydrostatic pressure, between 400 MPa and 600 MPa. Even though the
77 confidence interval of the individual pressure measurement by the sensor they
78 used was ± 16 MPa, as specified by the authors themselves, the fact that they used
79 multiple sensors in their experiments allowed them to reach the conclusion.

80

81 There have been numerous experimental studies to quantify and correlate
82 mechanical stress in the form of either pressure or shear, to cell mortality or
83 physical damage. **Perrier-Cornet et al. (1995, 1999)** used experimental
84 characterization to relate permeability of cell walls in yeast cells subjected to high
85 hydrostatic pressure. **Pagán and Mackey (2000)** studied the effect of pressure on
86 membrane damage in various strains of *E. coli* bacteria. It was observed that the
87 mechanism of inactivation is dependent on the level of pressure and the nature of
88 cell membrane damage may differ between species and phases of growth.
89 **Shimada et al. (1993)** observed mechanical damage to the mitochondria and
90 nuclear membrane of *Saccharomyces cerevisiae* after HPP at 400 MPa – 600 MPa
91 for 10 min. **Fernandes et al. (2001)** observed large differences in the
92 morphological changes after HPP between trehalose-6-phosphate synthase
93 mutants and wild-type *Saccharomyces cerevisiae*. **Moussa et al. (2013)** studied
94 the relationship of inactivation of *Saccharomyces cerevisiae* and volume
95 compression due to application of high hydrostatic pressure and found a critical
96 volume compression of $10 \mu\text{m}^3$ needed for cell inactivation. **Bulut et al. (1999)**

97 observed a non-trivial effect of shear and thermal forces on the microbial
98 inactivation of *Microbacterium lacticum*, and concluded that shear forces played a
99 larger role in inactivation than heat.

100

101 Numerical simulation has been used to study the stresses produced in
102 microbial cells during HPP and shed light on the understanding of cell
103 inactivation. **Hartmann and Delgado (2004a, 2004b)** used numerical simulation
104 to quantify the stresses occurring within yeast cells during high pressure
105 processing, and determined a critical Von Mises stress in the cell wall upon
106 failure between 415 MPa and 460 MPa. **Hartmann et al. (2006)** developed a
107 nonlinear model of a yeast cell under high pressure and showed different type of
108 stress conditions between the cell wall and the cytoplasm. **Otero and Sanz (2003)**
109 provided reviews of numerical models for heat transfer in HPP products at sub-
110 zero processing conditions. **Guignon et al. (2014)** determined density, specific
111 volume, isothermal compressibility and thermal expansion coefficient of whole
112 and skim milk between 0 °C and 60 °C and up to 350 MPa to allow future process
113 modeling.

114

115 We focus here on simulating the stress generated inside solid materials
116 due to the application of high hydrostatic pressure on the surface using a neo-
117 Hookean model, and how hard inclusions affect the internal stress distribution.

118 Neo-Hookean models have been used previously to study large deformations of
119 food materials (**Rakesh and Datta, 2011**) and polymeric materials (**Chen and**
120 **Lagoudas, 2008**). The stress at any point can be split into effective pressure and
121 shear, which cause volume change and deformation, respectively.
122 Mechanistically, each of these components may play a role during microbial
123 inactivation.

124

125 Preliminary experimental work was done with chicken and turkey
126 drumsticks, raw and cooked, to take advantage of the system of meat wrapped
127 around a bone. A bacterial inoculum in sodium alginate was injected at different
128 positions in the meat and gelled with calcium chloride, high pressure processed,
129 and enumerated. Unfortunately, there was high variability in the results since the
130 inocula could not be fixed at consistent locations between experiments, even by
131 gelling it. Moreover, each drumstick had a different meat and bone geometry, and
132 the meat had layers of muscle and fat tissue which was reflected in Young's
133 modulus measurement with over 28% variability (data not shown). Details of
134 these experiments can be found in **Maldonado (2016)**.

135

136 Since our work is aimed at exploring the pressure non-uniformity in
137 heterogeneous systems and not in any particular food system, we used a model
138 system to control for the natural variability of food materials. Our findings on the

139 development of pressure gradients in soft materials with hard inclusion during
140 high pressure processing still apply to a large extent to food materials.

141

142 **2. Theory**

143 In this section a review of the computational modeling aspects and the
144 material model to simulate stress distribution are presented.

145

146 2.1 Pressure as a Component of Stress

147 The physical quantity known as stress is a representation of forces
148 manifesting within the body in order to equilibrate with an externally applied
149 load(s). The components of stress are arranged in a square matrix, called the stress
150 matrix or stress tensor (σ), which is used in mathematical modeling and numerical
151 methods. The main diagonal of the matrix contains the normal stresses, and the
152 remaining elements are the shear stresses.

$$153 \quad \sigma = \begin{bmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{bmatrix} \quad (1)$$

154

155 Since it is difficult to easily interpret the physical significance of the
156 components of the stress-tensor, several invariant scalar measures of the stress-
157 tensor have been defined in-order to quickly characterize the nature of the force
158 distribution within a solid. The most significant of these measures are the

159 hydrostatic pressure component (p), which is intimately related to volume change
 160 of a specimen, and the effective stress deviator also known as the Von Mises
 161 stress (σ_{VM}), responsible for shape changes (Bower, 2010; Solecki and Conant,
 162 2003).

$$163 \quad p = \frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) \quad (2)$$

$$164 \quad \sigma_{VM} = \sqrt{\frac{(\sigma_{xx}-\sigma_{yy})^2 + (\sigma_{yy}-\sigma_{zz})^2 + (\sigma_{zz}-\sigma_{xx})^2 + 6(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{zx}^2)}{2}} \quad (3)$$

165

166 2.2 Mathematical Model for Stress Distribution

167 The stress developed inside a material is a function of the material
 168 properties of the specimen and the strain that the material is subjected to. For a
 169 linearly elastic isotropic material the stress tensor “ $\boldsymbol{\sigma}$ ” is written in terms of
 170 material constants (also known as Lamé constants) λ , μ , and the components of a
 171 strain tensor “ $\boldsymbol{\epsilon}$ ” as follows:

$$172 \quad \boldsymbol{\sigma} = \lambda e \mathbf{I} + 2\mu \boldsymbol{\epsilon} \quad (4)$$

173 Where, the scalar quantity

$$174 \quad e = \epsilon_{11} + \epsilon_{22} + \epsilon_{33} \quad (5)$$

175 is also known as the volumetric strain measure in small deformation and $\mathbf{I}$ is the
 176 second-order identity tensor. All tensorial quantities are bold-faced to distinguish
 177 them from scalar valued functions and variables. The Lamé constants λ and μ can

178 be written in terms of material properties, namely, the Young's modulus (E) and
179 the Poisson's ratio (ν), which can be determined using standardized mechanical
180 tests. The parameters λ and μ are given as follows:

$$181 \quad \lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \quad (6)$$

$$182 \quad \mu = \frac{E}{2(1+\nu)} \quad (7)$$

183 where, μ is the engineering shear modulus (also known as G). Another material
184 parameter of significance for deformable solids is the bulk modulus K ,

$$185 \quad K = \frac{E}{3(1-2\nu)} \quad (8)$$

186

187 The parameter " ν " is defined as the negative of the ratio of longitudinal
188 elongation of the material to the transverse contraction (for positive value of ν) or
189 expansion (for negative ν) when the material is stretched along the longitudinal
190 direction. Most materials (including meat, bone, etc.) have positive values of ν .

191 As the value of ν approaches 0.5 the value of K approaches infinity, or in
192 other words the material becomes incompressible, even though the shear modulus
193 G remains bounded. For a compressible solid subjected to external pressure, the
194 shear in the specimen will depend on G while the pressure developed will be
195 dictated by values of K . In the sections to follow the effects of these parameters
196 on the stress distribution inside the specimen are examined in detail.

197

198 The constitutive behavior given by eq. (4) is a widely accepted model for
199 most materials within limits of small deformation, beyond which most materials
200 deviate from a linear stress-strain relation. It is widely known that at higher
201 deformation levels the stress-strain behaviors of most materials are never linear.
202 Microstructural mechanisms such as damage, internal structural re-arrangement,
203 plasticity, etc. have been known to facilitate non-linear deformation of the
204 material. In this work we assume that the material remains elastic after
205 deformation and that the material returns to its original (undeformed) “stress-free”
206 state when the load on it is released. However, description of the inherent large
207 deformation kinematics requires the introduction of other tools. Continuum
208 mechanics provides the foundation for a mathematically correct description of
209 large or finite deformation processes in a material. The rest of this section will be
210 devoted the description of stress state within a material as it undergoes continuous
211 and large (but finite) deformation.

212

213 In a continuous displacement field, the deformations are described with
214 recourse to the analytical deformation gradient:

215
$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} \tag{9}$$

216 where $\mathbf{x}(\mathbf{X},t)$ (with components x_1, x_2, x_3) is the deformed vector coordinate of a
 217 material point originally located at $\mathbf{X}$ (with components X_1, X_2, X_3) in the un-
 218 deformed (or reference) coordinates. Eq. (9) can be written alternatively in terms
 219 of the individual components of the tensor $\mathbf{F}$ as,

$$220 \quad F_{ij} = \frac{\partial x_i}{\partial X_j} \quad (10)$$

221 where, i and j are numbers which can take the value of 1, 2 or 3. Just as the case
 222 of linear elasticity, the kinematic description introduced above (eq. 10) can be
 223 used to determine the stress state within a material undergoing finite deformation
 224 in terms of the strain measures defined above. The mathematical link between
 225 stress and strain is through constitutive response. For the case of a neo-Hookean
 226 material, the constitutive relations are derived from a strain energy potential of a
 227 particular functional form, usually written as:

$$228 \quad \psi \equiv \psi(\mathbf{C}) = \psi(I_C, II_C, III_C) \quad (11)$$

229 where I_C , II_C and III_C are a set of scalar invariant measures of the right Cauchy
 230 green deformation tensor, $\mathbf{C}$ (where, $\mathbf{C} = \mathbf{F}^T \mathbf{F}$) given as:

$$\begin{aligned} I_C &= I_B = tr(\mathbf{C}) = C_{11} + C_{22} + C_{33} \\ 231 \quad II_C &= II_B = \frac{1}{2}(I_C^2 - I_{C^2}) \\ III_C &= III_B = \det(\mathbf{C}) = \det(\mathbf{F})^2 = J^2 \end{aligned} \quad (12)$$

232 where, I_{C^2} is the trace of tensor $\mathbf{C}^2$, $tr(\mathbf{C}^2)$. The determinant “ J ” of the deformation
 233 gradient in eq. (9) is the ratio of local volume of the deformed body to that of the

234 un-deformed body. Hence, $J=1$ implies no volume change in the material after
235 deformation.

236

237 The internal stress can be calculated by taking the derivatives of the
238 energy function with respect to the tensor $\mathbf{C}$. Specifically, the Cauchy stress
239 tensor, which is the ratio of forces in the deformed configuration per unit area of
240 the *deformed* configuration, can be obtained from the energy functional using the
241 equation:

$$242 \quad \boldsymbol{\sigma} = J \mathbf{F} \frac{\partial \psi}{\partial \mathbf{C}} \mathbf{F}^T \quad (13)$$

243 where, $\mathbf{F}$ is the deformation gradient defined in eq. (10). It should be noted that
244 the Cauchy stress or true stress “ $\boldsymbol{\sigma}$ ” is the actual measure of stress developed in
245 the specimen undergoing deformation. Furthermore, for the limiting case of small
246 deformation for an isotropic elastic material, the Cauchy stress will reduce to eq.
247 (4).

248

249 2.3 Finite Deformation Models

250 In order to capture the non-linear behavior of bio-materials at finite
251 deformations, the analysis in this work assumes a non-linear elastic and isotropic
252 neo-Hookean material model. Isotropic neo-Hookean models can be defined in
253 terms of parameters that are closely related to the bulk modulus K (eq. 8) and

254 shear modulus μ or G (eq. 7). Specifically, the strain-energy density of a neo-
 255 Hookean material is assumed to have the following functional form:

$$256 \quad \Psi(\mathbf{C}) = \{KU(J) - G \ln J\} + \{0.5G(I_c - 3)\} \quad (14)$$

257

258 As seen in eq. (14), the deformational energy for an isotropic neo-
 259 Hookean model can be split in terms of a volumetric (or dilatation, term I inside
 260 the first set of brackets) and shape change (or deviatoric, term II in the second set
 261 of brackets) response. The energy density is defined in terms of invariant
 262 measures of the deformation tensor $\mathbf{C}$ (eq. (12)). Using the chain rule of
 263 differentiation, the Cauchy stress for this system can be derived to be:

$$264 \quad \boldsymbol{\sigma} = \frac{1}{J} \left[\left(KJ \frac{\partial U}{\partial J} - G \right) \mathbf{I} + G\mathbf{B} \right] \quad (15)$$

265 where, $\mathbf{B}$ is the left Cauchy deformation tensor (defined as, $\mathbf{B}=\mathbf{F}\mathbf{F}^T$). The
 266 following identities were used in the derivation of eq. (15):

$$267 \quad \frac{\partial I_c}{\partial \mathbf{C}} = \mathbf{I}$$

$$268 \quad \frac{\partial II_c}{\partial \mathbf{C}} = I_c \mathbf{I} - \mathbf{C} \quad (16)$$

$$269 \quad \frac{\partial III_c}{\partial \mathbf{C}} = III_c \mathbf{C}^{-1} = J^2 \mathbf{C}^{-1}$$

270 where, $\mathbf{C}^{-1}$ indicates the inverse of tensor $\mathbf{C}$.

271

272 If the parameters K and G are known and a suitable function is chosen for
 273 $U(J)$, then the stress developed inside the body can be computed using eq. (15). In
 274 practice, the material constants are determined from the small deformation range
 275 (i.e., the range in which stress-strain behavior remains fairly linear or Hookean)
 276 and the non-linearity is then accounted for by choosing an appropriate energy
 277 function, $U(J)$. However, it is usually difficult to estimate the functional
 278 parameters using experimental data.

279

280 2.4 Implications of Including Large Deformation Kinematics

281 The implications of including large deformation kinematics in the material
 282 model are now demonstrated using an example. Consider a uniaxial bar (for the
 283 sake of demonstration we consider that $\nu=0$) being extended uniformly in one-
 284 direction (see Fig. 1). Analytical solutions for the stress in the material can be
 285 derived to be of the form for the isotropic material to be:

$$286 \quad \sigma = E\varepsilon \quad (17)$$

287

288 Setting $\nu=0$, and $F_{11}=1+\varepsilon$, $F_{22}=F_{33}=1$ and $F_{ij}=0$ when $i \neq j$ in eq. (10), the stress in
 289 the Neo-Hookean material model would be:

$$290 \quad \sigma = E^* \frac{dU}{dJ} + E^* \frac{\varepsilon(\varepsilon+2)}{(\varepsilon+1)} \quad (18)$$

291 where ε is the ratio of end displacement to the original length of the material and
 292 $U(J)$ is a functional form for the bulk behavior of the material as function of the
 293 volume deformation metric J (in this example, $J=1+\varepsilon$). The term E^* is used to
 294 emphasize the fact that the material constant is determined from the small
 295 deformation limit of eq. (18) and is not necessarily the same value as Young's
 296 modulus 'E'. Specifically, in the limit of small deformation (i.e. in the limit $\varepsilon \rightarrow 0$),
 297 the value of E^* for model 1 through 3 (eq. 19-21) was determined to be $3E$, while
 298 for model 4 is $4E$. Fig. 2 is the stress developed in the model predicted due to
 299 simple linear elasticity compared to non-linear models (1 through 4) in which the
 300 functional forms for $U(J)$ were as follows:

$$301 \quad U_1(J) = \frac{1}{4}(J^2 - 1 - 2 \ln J) \quad (19)$$

$$302 \quad U_2(J) = \frac{1}{2}(J - 1)^2 \quad (20)$$

$$303 \quad U_3(J) = \frac{1}{2}(\ln J)^2 \quad (21)$$

$$304 \quad U_4(J) = 2(J - 1 - \ln J) \quad (22)$$

305

306 We see that at small deformations, the linear elastic Hooks law behavior
 307 of the material is recovered. On the other hand, at large deformations the interplay
 308 functional forms of $U(J)$ and second term in eq. (18) dominate the stress response
 309 of the neo-Hookean models. Fig. 3 for example, depicts the relative contribution
 310 of the first term of eq. (18) to the total stress. Quite clearly, the linear model will

311 be unable to accurately represent the constitutive response of non-linear material
312 systems. However, the choice of function for the neo-Hookean model must be
313 representative of the physics of the system at large deformation as it would have a
314 large impact on the accuracy of the model.

315

316 In this work, a neo-Hookean material model was developed to simulate the
317 constitutive response of the gel-system used to simulate a food material. The
318 material models were developed and implemented in the commercial finite
319 element code ABAQUS (Dassault Systèmes, Vélizy-Villacoublay, France), using
320 the UHYPER user-subroutine.

321

322 **3. Materials and Methods**

323

324 **3.1 Experimental measurement of mechanical properties**

325 Experiments were carried out to characterize a model food system to
326 determine realistic values of material properties needed for the numerical
327 simulations. A model system comprising of a 3% agar hydrogel was designed to
328 simplify the material properties for stress distribution simulations and to assure
329 that the future experimental stage would be consistent (real food systems, like
330 turkey or chicken drumsticks, would have different bone sizes and orientations,
331 and meat thickness).

332

333 The gel was made using RS-100 agar powder (TIC Gums, MD, USA),
334 which was boiled, poured in a plastic bottle, and left to set in a refrigerator for
335 approximately 24 hours. Fig. 4 shows a schematic of the model system.

336

337 The compressibility of the gel was measured at high pressures in order to
338 validate the model. A block of agar gel, between 10 g to 13 g, was inserted into a
339 26 mL tabletop high-pressure vessel (Elmhurst Research, Inc., NY, USA), shown
340 in Fig. 5; the remaining volume was filled with water. The vessel was pressurized
341 using a Carver model K manual press (Carver, Inc., IN, USA), which was used to
342 insert a piston into the vessel. The position of the piston, monitored using an IL-
343 1000 LVDT sensor (Keyence, IL, USA), was used to calculate the volume of the
344 inserted piston length, which would correspond to the compression of the water
345 and sample inside the vessel, and also the compression of other elements such as
346 the seals and the pressure sensor. In order to account for the compression of these
347 additional elements inside the vessel, our data for density of water at different
348 pressures was compared to the density of water from the National Institute of
349 Standards and Techniques (NIST) data (**Harvey et al., 2010**), compiled from the
350 works done by **Grindley et al. (1971)** and **Hilbert et al. (1981)**. The calculated
351 compression beyond the expected based on the NIST data was assumed to be
352 those additional elements.

353

354 3.2 Numerical Simulation

355 The compression data of the gel was used to determine a suitable model
356 for the function $U(J)$, so eq. (17) could be used to simulate the stress profile inside
357 the gel during HPP. The bulk modulus in eq. (17) was obtained from the NIST
358 data for compression data of water at 0.1 MPa of pressure, since the gel was 97%
359 water. In order to validate the use of the compression data for the gel, it was
360 compared to the NIST data for compression of water.

361

362 Following eq. (2), the pressure field inside the neo-Hookean material
363 (based on the model given in eq. (15)) would be:

$$364 \quad p = -\frac{\sum_{i=1}^3 \sigma_{ii}}{3} = -\left[K \frac{\partial U}{\partial J} + \frac{G}{J} \left\{ \frac{\sum_{i=1}^3 B_{ii}}{3} - 1 \right\} \right] \quad (23)$$

365

366 For a unit cube undergoing isotropic compression (see Fig. 6) the
367 analytical solution for pressure in the neo-Hookean solid² would be:

$$368 \quad p = -\left[K \frac{\partial U}{\partial J} - G \frac{\Delta(2-\Delta)}{(1-\Delta)^3} \right] \quad (24)$$

369

² The analytical solution can be derived by substituting $F_{11}=F_{22}=F_{33}=1-\Delta$ (isotropic compression) and $F_{ij}=0$ when $i \neq j$) in eq. (18)

370 In the previous section, we had shown that in neo-Hookean material
 371 models the stress developed at large deformations depends on the functional form
 372 of $U(J)$. In order to determine it, the shear modulus and the functional form of
 373 $U(J)$ were calibrated to match the experimental pressure vs. volume change curve.
 374 Since the shear modulus for the material is extremely low (the gel was 97%
 375 water), the first term in eq. (18) becomes the dominant term in pressure response
 376 of the proposed material model.

377
 378 It was seen through trial and error of models 1 through 4 that a function of
 379 the form $\frac{dU}{dJ} = \frac{\ln J}{J^A}$ would be a viable candidate in the choice for $U(J)$ in the
 380 proposed neo-Hookean material model (setting $A=1$ would produce model 3, eq.
 381 (21)). Setting $A=3.5$ seemed to capture the experimental pressure-volume change
 382 curve quite well. (see Fig. 7). Fig. 7 shows the comparisons of experimental data
 383 with numerical predictions when the $U(J)$ is changed from models 1 through 4.
 384 The final form selected was:

$$385 \quad U(J) = -\frac{2}{5} \frac{\ln J}{J^{2.5}} - \frac{4}{25} \left(\frac{1}{J^{2.5}} - 1 \right) \quad (25)$$

386
 387 With the above form, the shear modulus (G) in eq. (23) was adjusted using
 388 linear search until a good fit to the experimental data for the compression of the
 389 3% agar gel was obtained. The value of K was fixed at 2.1 GPa. The shear

modulus was determined to be 4.6 kPa. The model for the bulk behavior of the gel under pressure was implemented as an extension to the current neo-Hookean models in ABAQUS. Substituting for $U(J)$ in eq. (15), the Cauchy stress for this model is derived as:

$$\boldsymbol{\sigma} = \left(K \frac{\ln J}{J^{3.5}} - \frac{G}{J} \right) \mathbf{I} + \frac{G}{J} \mathbf{B} \quad (26)$$

The hard inclusion (wood) was assumed to have $E = 20$ GPa and $\nu = 0.3$. Typically, the modulus of wood varies between 6 GPa and 20 GPa and the Poisson's ratio between 0.4 and 0.25 depending on the type of wood, environmental conditions, age, etc. (Ross, 2010; Kretschmann, 2010). These values are close to the published mechanical properties of bone (Zysset et al., 1999; Bosisio et al., 2007), which made wood a good surrogate for our work with the added advantage over natural bone that the geometry can be kept constant between experiments. Wood is naturally orthotropic, i.e., material properties vary as a function of material orientation (e.g. how fibers are oriented within the wood specimen). For the purposes of this work, the hard inclusion was simplified to be isotropic in nature and conservatively stiffer. Pressurization experiments on the composite gel-wood showed elastic deformation on both the gel and the wood. No change in volume or shape, besides some minor tears in the gel at the interface with the wood, were observed after a pressurization cycle.

410

411 Hydrostatic pressure was applied perpendicularly on the external surfaces.

412 The inherent symmetry of the model allowed for an axi-symmetric (about the
413 cylinder axis) analysis of the model. The symmetry in load application allowed
414 for further simplification of the analysis model. The governing equations for a
415 deformable solid object were solved using finite element analysis (FEA), which
416 was needed to quantify the stress field in a non-linear material model. The finite
417 element analysis code ABAQUS (Dassault Systèmes, Vélizy-Villacoublay,
418 France) and user-deployed subroutines were used to implement the proposed neo-
419 Hookean material model which were then used in all simulations.

420

421 Finite Element Analysis (FEA) solutions are dependent on the level of
422 discretization mesh, especially in areas where appreciable stress/strain gradients
423 are expected to occur. Coarse meshes can result in unreliable results and introduce
424 spurious uncertainty into simulation predictions. In this work, in order to verify
425 that the numerical solution was not affected by choice of discretization, three
426 meshes of increasing grid density were employed in the analysis, show in Fig. 8.
427 The mesh was progressively refined inside the gel area to characterize the
428 dependence of the solution on mesh geometry. While the finite element mesh

429 around the wood insert was fixed at 14×63^3 , the mesh in the gel was
430 progressively refined from 52×63 (Mesh 1), 104×63 (Mesh 2) and 156×63 (Mesh
431 3) elements in the radial (R) and axial (Z) directions, respectively.

432

433 **4. Results and Discussion**

434 Fig. 9 shows the comparison of the experimental data for the compression
435 of the gel and a plot of eq. 26. The coefficient of determination (R^2) was 0.974,
436 which indicates that the model accurately described the behavior of the gel. The
437 coefficient of determination of the comparison between the compressibility of the
438 gel and the compressibility of water based on NIST data was 0.973, indicating
439 also high degree of correlation. These validated the use of the physical properties
440 of water at atmospheric pressure in the neo-Hookean model of the gel.

441

442 Due to the near incompressibility of the gel material, spurious pressure
443 gradients can cause numerical artifacts such as element locking (**Bathe, 1996**). In
444 this work, specialized mixed formulation elements were adopted to circumvent
445 this issue. An extensive treatise on numerical locking and its related numerical
446 instabilities as well as the suggested work-around has been discussed in detail in
447 in **Bathe (1996)**. The numerical procedure for solving the gel system followed an

³ Nomenclature indicates 14 elements in R direction 63 elements in Z direction, which results in element size of 0.564 mm x 0.603 mm

448 iterative strategy in which the load (in this case the pressure on the gel system)
449 was gradually increased in successive steps until its full value (300 MPa).

450

451 Fig. 10 shows the results of the FEA simulations of stress distribution in
452 the gel with a hard inclusion when high pressure (300 MPa) is applied at the
453 surface. The various colors depict the variation of pressure and Von Mises stress
454 along the mid-plane of the 2D model for all three choices of mesh discretization.
455 Because the material is nearly incompressible (ν is very close to but not equal to
456 0.5), the pressure field is almost uniform throughout the material domain. A
457 negligibly small gradient in the pressure field occurs near the interface between
458 the gel and the wooden inclusion. This implies that microorganisms within the
459 gel and away from the inclusion would be subjected to a uniform hydrostatic
460 pressure. The effective Von Mises stress near the insert does not increase to a
461 significant level due to the relatively small shear modulus of the gel.

462

463 Shown in Fig. 11 and 12 are contours of hydrostatic pressure and Von
464 Mises stress distribution, respectively, for each case of mesh discretization. A
465 clear convergence of contours and point-wise numerical predictions for all three
466 cases of discretization is observed. The finer mesh is also able to resolve the
467 interfacial features of the stress field near the gel-wood interface which is crucial

468 to the thesis of this work. The results demonstrate the invariance of simulation
469 prediction on discretization.

470

471 In order to test the effect of different material properties, the simulations
472 (using mesh 3 from Fig. 8) were carried out for different values of Poisson's ratio
473 (ν) in the gel material. The pressure and shear stress profiles are shown in Fig. 13.
474 Based on eq. (7), as Poisson's ratio decreased from 0.5 (incompressible solid)
475 towards 0, the shear modulus (μ or G) of the material increased, which would
476 cause a higher shear stress to be developed toward the hard inclusion and a
477 steeper pressure gradient in the material. For example, at $\nu=0.2$ a microbial cell
478 near the hard inclusion would sustain 285 MPa of pressure and 70 MPa of shear
479 vs. a cell on the surface that would sustain only 300 MPa of pressure and close to
480 zero shear. **Segars et al. (1977)** determined that Poisson's ratio of beef was
481 between 0.2 and 0.26. These values were obtained at atmospheric pressure so they
482 cannot be fully reliably used for our simulations at high pressure (for example,
483 our measurements of the bulk modulus of the gel at high pressure was 3.2 GPa,
484 compared to the value at atmospheric pressure of 2.1 GPa).

485

486 Solid food materials are generally heterogeneous, either at a macroscopic
487 (for example, meat with bones or particulates) or microscopic (for example, starch
488 granules) level. The micro-structures of such materials are usually a composite of

489 hard inclusions (with large bulk modulus) embedded in a soft matrix (with low
490 bulk modulus). The effectiveness of HPP for microbial inactivation depends
491 entirely on the stress fields that can be generated within the material and
492 effectively applied on the microorganisms inside. From Fig. 13 it is evident that
493 the presence of heterogeneities could affect the stress distribution in the material
494 quite dramatically. In particular, in compressible solids with inclusions, the
495 presence of those inclusions could cause significant shearing and lower pressures
496 at or near the interfaces between the compressible solid and the inclusions,
497 depending on the mechanical properties of the materials. These predicted results
498 do not support the prior assumptions that the pressure is always uniform in
499 materials during HPP. From the results above, it is sufficiently clear that pressure
500 distribution in solid foods can be assumed to be uniform only in cases when the
501 material behavior is extremely close to the incompressible limit.

502

503 Clearly, as the material deviates from near incompressibility (i.e., $\nu \sim 0.5$)
504 the values of shear become comparable to the applied pressure in the specimen. It
505 is possible that certain forms of microorganisms are more susceptible to shear
506 while there might be others that are inactivated by pressure (**Perriere-Cornet**
507 **1995 and 1999; Pagán et al., 2000; Bulut et al. 1999**). It might be also beneficial
508 to look at a combination of pressure and shear that might play a synergistic or
509 antagonistic role in microbial inactivation. There might be an optimal value of

510 P/σ_{VM} for which maximum inactivation can be achieved. These optimum
511 conditions may also translate into a lower applied overall pressure on the system
512 and hence lower expended energy, resulting in an energy efficient alternative to
513 regular HPP.

514

515 **5. Conclusions**

516 It was shown that a fundamental understanding of the mechanical
517 properties of food materials is essential in understanding the internal distribution
518 of stresses during HPP, and that the internal stresses may not necessarily be
519 uniform as it has been assumed. It was shown that the stress distribution is
520 dependent on a) the heterogeneities of the HPP material system and b) the
521 compressibility of the material specimens. Further, since the inactivation is driven
522 by the applied stress on the bacterial cell, better material models are required to
523 study how material properties affect microbial inactivation in high pressure
524 processing. It has also been argued that a better understanding of the inactivation
525 criteria for a particular kind of microorganisms via susceptibility to shear and/or
526 pressure allows for a better design of experiments such that the HPP procedure is
527 effective in achieving the desired inactivation levels at all locations inside a solid
528 food material.

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651 by nanoindentation in the human femur. J Biomech, 32 (10), 1005-1012.

652

653 Figure 1: Demonstrative example: Uniaxial tension of a bar (with no Poisson's
654 effect).

655

656 Figure 2: Comparison of predictions of stress as a function of strain for a linear
657 elastic model and four (4) non-linear models (eq. 19 – 22).

658

659 Figure 3: Relative contribution of the first term of eq. (18) to the total stress, for
660 the different forms of $U(J)$

661

662 Figure 4: Schematic of the model system. The grey section represents the wood
663 inclusion and the white section the gel material.

664

665 Figure 5: Tabletop high pressure vessel (26 mL capacity) on a hydraulic press.

666

667 Figure 6: Cube undergoing isotropic compression.

668

669 Figure 7: Trial and error process for determining the $U(J)$ function of the neo-
670 Hookean model for the gel system.

671

672 Figure 8: Mesh used for finite element analysis of stress distribution during high
673 pressure processing. a) Mesh 1, 52x63 elements in gel (52 along R-axis and 63

674 along Z-axis). b) Mesh 2: 104x63 elements (104 along R-axis and 63 along Z-
675 axis). c) Mesh3: 156x63elements (156 along R-axis and 63 along Z-axis).

676

677 Figure 9: Verification of numerical implementation of eq. (26) with analytical
678 predictions and experimental data for bulk behavior of gel.

679

680 Figure 10: Results of the FEA simulation along the mid-plane of symmetry of the
681 model system. The hard inclusion is on the left side of the graph, the surface of
682 the gel where pressure was applied is on the right side.

683

684 Figure 11: Contour plots of hydrostatic pressure distribution in the model system.
685 a) Mesh 1 (coarsest). b) Mesh 2. c) Mesh 3 (finest).

686

687 Figure 12: Contour plots of shear stress distribution in the model system. a) Mesh
688 1 (coarsest). b) Mesh 2. c) Mesh 3 (finest).

689

690 Figure 13: Effect of Poisson's ratio on hydrostatic pressure and shear stress
691 distribution in the model system.

Poisson ratio, $\nu=0$

Figure 2

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7

Figure 8a

Figure 8b

Figure 8c

Figure 9

Figure 10

Figure 11a

Figure 11b

Figure 11c

Figure 12a

Figure 12b

Figure 12c

Figure 13