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RESEARCH ARTICLE

Validation of a heterogeneous elastic-biphasic model for the numerical simulation of the PDL

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An elastic-biphasic model for the simulation of the periodontal ligament (PDL) and the adjacent tooth is presented and investigated. The PDL is modelled as a biphasic material following the work of Ehlers and Markert (2001) whereas the tooth is modelled as a linear elastic body. A spatial discretisation scheme is proposed based on mixed finite elements for the spatial discretisation. Due to non-linearity in the model, a predictor-corrector scheme is employed as a temporal discretisation scheme. In order to validate the PDL model in-vitro measurements are compared to numerical simulations. The numerical simulations are performed using geometries resulting from μ-CT of the same porcine tooth which was employed for the in-vitro measurements.

Keywords: finite elements; biphasic theory; periodontal ligament; elastic-biphasic coupling; partial differential equation

1. Introduction

The numerical simulation of biological materials is a demanding task. This is due to the inherent complexity of many biological materials, which often are strongly heterogeneous in nature. This holds in particularly true for the periodontal ligament (PDL), which is a thin layer of dense soft connective tissue located between tooth root and the jaw bone (see Berkowitz et al. (2009) for a detailed description). The PDL consists of a solid phase, formed by collagen fibres, and a liquid phase, filling up the tissue with interstitial liquid. As a consequence, any mathematical model which might be employed for the numerical simulation of the PDL, should take the biphasic nature of this material into account. In particular, the model should be able to render the elastic behaviour of the solid phase as well as the incompressible nature of the mixture constituting the PDL.

Mathematical models for biphasic materials are well-known in engineering related applications such as ground water flow (Verruijt 1970). On the other hand, in the last decades biphasic materials were also employed in the context of biological materials. For example Mow and Hung (2001) and Ehlers and Markert (2001) used it to model the mechanical behaviour of cartilage.

However, a challenge in modelling the mechanical behaviour of the PDL are the stresses induced by the interstitial liquid and the incompressible nature of the PDL. To this end, the PDL often is modelled by anisotropic, non-linear or viscoelastic material laws. In particular, some of these models describe the incompressible nature of the PDL employing a "penalty term", e.g. (Pietrzak et al. 2002). On the

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other hand, Natali et al. (2007) proposed a nonlinear anisotropic material law in order to take the orientation of the collagen fibres into account. A third class of models aims for the description of the temporal (non-linear) stress-strain relationship in the PDL employing viscoelastic laws, see for instance (Toms et al. 2002; Justiz 2004). In these models the influence of the interstitial liquid is implicitly given by means of abstract material parameters which can be adjusted in order to improve the approximation strength of the numerical simulations to the outcome of in-vitro measurements.

In the present article, we propose the (to our knowledge new) idea of using biphasic materials for the mathematical modelling and numerical simulation of the PDL. As we will describe, the employed biphasic model is a "smeared model" which explicitly takes the fibres-fluid ratio into account, as described by Ehlers and Markert (2001). Beside this, also the incompressible nature of the material is described.

To this end, we will present a biphasic model for the application in the context of PDL simulations. In particular, we will derive a coupled biphasic-elastic model describing the behaviour of a tooth and its surrounding PDL under external loading conditions. In our context, we model the tooth as a second domain where a linear elastic material law is applied. In this article we are in particular concerned with the numerical results to in-vitro measurements of porcine teeth for which we employ the same, realistic three-dimensional porcine geometries obtained by μ-CT scans.

2. Mathematical Modelling

As pointed out before, the PDL can be interpreted as a biphasic material, which is formed by a fibrous network of collagen, surrounded by interstitial fluid. Therefore, in this section we describe the biphasic model which is employed for modelling the PDL.

The basic idea of the biphasic theory is to use a macroscopic approach, which is not resolving the complicated micro-structure of the collagen fibres. Instead, the material is modelled as the mixture of a homogeneous solid S and a fluid F, which are both assumed to coexist at each material point. The relative volume fractions n^S and n^F then specify the local composition of the material. Thus, all quantities, such as deformations or stresses, exists for both the fluid and the solid phase. Both the collagen and the fluid then influence the stress response of the biphasic material.

In the present article, we are following an approach presented in the context of porous media, which goes back to the work of Bowen (1976, 1980). During the last decades, these ideas have been extended and employed in the framework of biological materials (Ehlers 1995; Ehlers and Markert 2001).

2.1 A Biphasic Model for the PDL

The model we will use for describing the mechanical behaviour of the PDL was first presented by Ehlers and Markert (2001). A fundamental assumption in mixture theory, on which the model is based, is the idea of superimposed continua: instead of geometrically resolving the liquid and solid distributions, the distributions are obtained by averaging over a representative volume. Therefore, instead of introducing a microscopic model, one assumes that at each material point both phases coexist. Therefore, we have to treat physical quantities associated to the respective phases separately and will thus introduce the superscripts ^{S} and ^{F} in

order to distinguish between them.

From the kinematical point of view, each material point $\boldsymbol{p} \in \Omega^{\mathrm{PDL}}$ is moving according to *two* deformations $\boldsymbol{\varphi}^S(\boldsymbol{p},t)$ and $\boldsymbol{\varphi}^F(\boldsymbol{p},t)$, where $\Omega^{\mathrm{PDL}} \subset \mathbb{R}^3$ denotes the PDL domain in its reference configuration. Here, we emphasize that in general we cannot expect that both deformations coincide, i.e., generally we have

$$\boldsymbol{x}^S = \boldsymbol{\varphi}^S(\boldsymbol{p},t) \neq \boldsymbol{\varphi}^F(\boldsymbol{p},t) = \boldsymbol{x}^F \qquad \boldsymbol{p} \in \Omega^{\mathrm{PDL}}, \forall t \in (0,T_f]$$

where T_f denotes the final simulation time. However, the image of the reference configuration Ω^{PDL} is the same under both deformations

$$\boldsymbol{\varphi}^S(\Omega^{\mathrm{PDL}},t) = \boldsymbol{\varphi}^F(\Omega^{\mathrm{PDL}},t) \quad \text{for all } t \geq 0.$$

cf. also Figure 1. Moreover, each component has its own velocity field

$$\dot{\boldsymbol{x}}^\alpha = \frac{\partial \boldsymbol{\varphi}^\alpha(\boldsymbol{p},t)}{\partial t}$$

Now, the local structure of the mixture is given by the volume fractions $n^\alpha = n^\alpha(\boldsymbol{x},t)$ ($\alpha \in \{S,F\}$) that describe the ratio of the fluid and solid phase at each spatial point $\boldsymbol{x}$. A fundamental assumption of the model is that no empty space is allowed between the phases, i.e., that the saturation condition

$$n^S + n^F = 1 \tag{1}$$

holds. Denoting by $\rho^{\alpha R}$ the realistic physical density of the phase α, its contribution to the total density therefore is $\rho^\alpha = n^\alpha \rho^{\alpha R}$.

The motion of the solid part is described in terms of the displacements $\boldsymbol{u}^S = \boldsymbol{\varphi}^S(\boldsymbol{p},t) - \boldsymbol{p}$. Furthermore, under normal loading conditions, only small strains will arise in the PDL. Thus, we can assume linear elastic behaviour of the solid part of the stress tensor, which allows us to use the linearised Green-St-Venant strain tensor, i.e.,

$$\boldsymbol{\epsilon}(\boldsymbol{u}^S) = \frac{1}{2}\left(\nabla \boldsymbol{u}^S + (\nabla \boldsymbol{u}^S)^t\right) \tag{2}$$

where A^t denotes the transposition operator of a tensor A. Within the framework of linear elasticity, the volume fraction $n^S = n_0^S / \det(\nabla \boldsymbol{\varphi}^S)$ of the solid part can be approximated as

$$n^S \approx n_0^S (1 + \nabla \cdot \boldsymbol{u}^S)^{-1} \approx n_0^S (1 - \nabla \cdot \boldsymbol{u}^S).$$

Furthermore, as a consequence of the saturation condition (1), we have

$$n^F = n_0^F + n_0^S \nabla \cdot \boldsymbol{u}^S.$$

Here n_0^S and n_0^F denote the initial volume fractions which satify the saturation condition.

The equation system describing the biphasic model is:

$$\begin{aligned} -\nabla \cdot \left(\boldsymbol{T}^S + \boldsymbol{T}^F\right) &= (\rho^S + \rho^F)\boldsymbol{g} && \text{on } \Omega^{\mathrm{PDL}} \\ \nabla \cdot \left(\dot{\boldsymbol{u}}^S - \zeta(n^F)\nabla p\right) &= -\nabla \cdot \left(\zeta(n^F)\rho^{FR}\boldsymbol{g}\right) && \text{on } \Omega^{\mathrm{PDL}} \end{aligned} \tag{3}$$

Here, $\rho^\alpha \boldsymbol{g}$ denotes the volume forces and $\zeta(n^F)$ is the deformation dependent Darcy parameter, proposed by Mow et al. (1982) as

$$\zeta(n^F) = \frac{k^F(n^F)}{\gamma^{FR}}\,. \tag{4}$$

Here the denominator is the effective fluid-solid specific weight

$$\gamma^{FR} = (\rho^S + \rho^F)\boldsymbol{g}$$

and the numerator is a power function that describes the influence of the permeability on the the fluid ratio

$$k^F(n^f) = k_0^F \left(\frac{n^F}{n_0^F}\right)^\kappa \tag{5}$$

where $\kappa > 1$ and k_0^F is the initial permeability.

Equation (3.1) is the linear momentum balance for the global mixture. Here, $\boldsymbol{T}^\alpha$ denotes the respective Cauchy stress tensors. Hassanizadeh and Graya (1980) showed that $\boldsymbol{T}^\alpha$ are symmetric if microscopically non-polar constituents are assumed. The Cauchy stress tensors can be written as

$$\boldsymbol{T}^\alpha = -n^\alpha p \boldsymbol{I} + \boldsymbol{T}_E^\alpha \tag{6}$$

where p is the effective fluid pressure. By neglecting frictional stresses in the fluid ($\boldsymbol{T}_E^F = 0$), the equilibrium of forces reads

$$-\nabla \cdot \left(\boldsymbol{T}_E^S - p\boldsymbol{I}\right) = (\rho^S + \rho^F)\boldsymbol{g}.$$

We note that in this equation the pressure p plays the role of a Lagrange multiplier for the incompressibility constraint. The equation (3.2) is derived by balances of mass for the two constituents and the Darcy law. Let us finally remark that $\zeta(n^F)$ is the only non-linear term present in the biphasic model (3).

2.2 Coupled Model for Tooth and Periodontal Ligament

We now complement the above introduced biphasic model for the PDL with a linear elastic model for the adjacent tooth. Our final aim is the formulation of a coupled model, which allows for describing the mechanical properties of the coupled PDL-tooth system. As we did for the PDL, we also identify the tooth in its reference configuration with the bounded domain $\Omega^{\text{Tooth}} \subset \mathbb{R}^3$ and denote all associated quantities with the superscript ^{T}. Starting from the equilibrium equation

$$-\nabla \cdot \boldsymbol{T}_E^T = \rho^T \boldsymbol{g} \quad \text{on } \Omega^{\text{Tooth}} \tag{7}$$

where $\boldsymbol{u}^T$ is the displacement vector on Ω^{Tooth}, i.e., on the tooth. We also impose the following compatibility conditions on the interface $\Gamma^I = \overline{\Omega^{\text{Tooth}}} \cap \overline{\Omega^{\text{PDL}}}$ between the tooth and the PDL:

$$\begin{aligned} \boldsymbol{u}^T &= \boldsymbol{u}^S && \text{on } \Gamma^I \\ \boldsymbol{T}_E^T \cdot \boldsymbol{\nu}^T &= -(\boldsymbol{T}_E^S - p\boldsymbol{I}) \cdot \boldsymbol{\nu}^{\text{PDL}} && \text{on } \Gamma^I \end{aligned} \tag{8}$$

Here, $\boldsymbol{\nu}^{\mathrm{PDL}}$ and $\boldsymbol{\nu}^{T}$ denote the outward normals to Ω^{PDL} and to Ω^{Tooth}, respectively. By exploiting the compatibility conditions (8), and equations (7) and (3), we obtain the following coupled system of PDEs for the PDL-tooth system

$$\begin{aligned} -\nabla \cdot \boldsymbol{T} &= \rho \boldsymbol{g} && \text{on } \Omega \\ \nabla \cdot \left(\dot{\boldsymbol{u}}^{S} - \zeta \nabla p\right) &= -\nabla \cdot \left(\zeta \rho^{FR} \boldsymbol{g}\right) && \text{on } \Omega^{\mathrm{PDL}} \\ \boldsymbol{u} &= \hat{\boldsymbol{u}} && \text{on } \Gamma^{D} \\ \boldsymbol{T} \cdot \boldsymbol{\nu} &= \hat{\boldsymbol{t}} && \text{on } \Gamma^{N} \\ \zeta(n^{F})(\nabla p - \rho^{FR} \boldsymbol{b}) \cdot \boldsymbol{\nu}^{PDL} &= f && \text{on } \partial\Omega^{\mathrm{PDL}} \end{aligned} \tag{9}$$

where $\Omega = \Omega^{\mathrm{Tooth}} \cup \Omega^{\mathrm{PDL}}$. In (9), we have also indicated by $\Gamma^{N} \subset \partial\Omega$ and $\Gamma^{D} \subset \partial\Omega$, $\overline{\Gamma^{N} \dot{\cup} \Gamma^{D} \dot{\cup} \Gamma^{I}} = \partial\Omega$, the Neumann and Dirichlet boundaries and by $\hat{\boldsymbol{u}}$ and $\hat{\boldsymbol{t}}$ the corresponding boundary values in equations (9.3) and (9.4). The function f denotes the flux of the fluid through the surface of Ω^{PDL}. Moreover, $\boldsymbol{u}|_{\Omega^{\mathrm{PDL}}} = \boldsymbol{u}^{S}$, $\boldsymbol{u}|_{\Omega^{\mathrm{Tooth}}} = \boldsymbol{u}^{T}$, $\Omega = \Omega^{\mathrm{PDL}} \cup \Omega^{\mathrm{Tooth}}$, are the displacements, p the fluid pressure, and $\boldsymbol{\nu}$ is the outward directed normal of Ω. In (9.1) the stress tensor $\boldsymbol{T}$ and the density $\boldsymbol{\rho}$ are defined as follows:

$$\boldsymbol{T} = \boldsymbol{T}(\boldsymbol{u}, p) = \begin{cases} \boldsymbol{T}_{E}^{T}(\boldsymbol{u}^{T}) & \text{on } \Omega^{\mathrm{Tooth}} \\ \boldsymbol{T}_{E}^{S}(\boldsymbol{u}^{S}) - p\boldsymbol{I} & \text{on } \Omega^{\mathrm{PDL}} \end{cases} \tag{10}$$

and

$$\rho = \begin{cases} \rho^{T} & \text{on } \Omega^{\mathrm{Tooth}} \\ \rho^{F} + \rho^{S} & \text{on } \Omega^{\mathrm{PDL}} \end{cases} \tag{11}$$

We also employ the symbol $\boldsymbol{T}_{E} = \boldsymbol{T}_{E}(\boldsymbol{u})$ to refer to the elastic part of the stress tensor $\boldsymbol{T}$.

Owing to our assumption of linear elastic materials, the Cauchy tensors $\boldsymbol{T}_{E}^{\alpha}$, $\alpha \in \{S, T\}$, can be written as

$$\boldsymbol{S}_{E}^{\alpha} = 2\mu^{\alpha} \boldsymbol{\epsilon}(\boldsymbol{u}) + \lambda^{\alpha} (\nabla \cdot \boldsymbol{u}) \boldsymbol{I} \tag{12}$$

where $\boldsymbol{\epsilon}(\boldsymbol{u})$ is the linearised strain tensor as defined in (2).

Let us remark that also anisotropic material laws can be employed in this framework, as long as $\boldsymbol{S}_{E}^{\alpha}$ is a symmetric tensor. Furthermore, in the context of the presented biphasic model, $\boldsymbol{T}_{E}^{S}$ might also render a non-linear or viscoelastic material law.

3. Discretisation in Space and Time

In order to carry out the numerical simulations and evaluation studies in Section 4.2, we have to discretise the coupled model (9). In the context of our coupled biphasic material laws, this means that we have to discretise the PDE in time and in space. Here, we employ the method of lines i.e., we first discretise the PDEs in space and then in time. However, Rothe's method might be employed as well, allowing for adaptively refining meshes from time step to time step.

Multiplying the first line of (9) with a sufficiently smooth vector valued test function $\boldsymbol{v}$ and the incompressibility constraint in the second line of (9) with the scalar test function q, we obtain after integration by parts the following weak

formulation of (3): find $(\boldsymbol{u}, p) \in (L^2((0,T_f];V) \times L^2((0,T_f];Q)$ such that

$$a(\boldsymbol{u},\boldsymbol{v}) - b(\boldsymbol{v},p) + b(\dot{\boldsymbol{u}},q) + c(p,q) = F(\boldsymbol{v}) + G(q) \tag{13}$$

for all $\boldsymbol{v} \in V$ and for all $q \in Q$, where $V = [H^1_{\Gamma_D}(\Omega)]^3$ and $Q = H^1(\Omega^{\mathrm{PDL}})$ and

$$\begin{aligned} a(\boldsymbol{u},\boldsymbol{v}) &= \textstyle\int_\Omega \boldsymbol{T}_E(\boldsymbol{u}) \colon \boldsymbol{\epsilon}(\boldsymbol{v})\, d\Omega \\ b(\boldsymbol{u},q) &= \textstyle\int_{\Omega^{\mathrm{PDL}}} \nabla \cdot \boldsymbol{u} q\, d\Omega \\ c(p,q) &= \textstyle\int_{\Omega^{\mathrm{PDL}}} \zeta \nabla p \cdot \nabla q\, d\Omega \\ F(\boldsymbol{v}) &= \textstyle\int_\Omega \rho \boldsymbol{b} \cdot \boldsymbol{v}\, d\Omega + \int_{\Gamma_N} \hat{\boldsymbol{t}} \cdot \boldsymbol{v}\, d\Gamma \\ G(q) &= \textstyle\int_{\partial\Omega^{\mathrm{PDL}}} f q\, d\Gamma + \int_{\Omega^{\mathrm{PDL}}} \zeta \rho^{FR} \boldsymbol{b} \cdot \nabla q\, d\Omega \end{aligned} \tag{14}$$

The weak formulation (13) is the basis for our discretisation in space and time which is done by means of low order finite elements in space and finite differences in time.

Since the two unknown functions $\boldsymbol{u}$ and p belong to the same functional space H^1 we can use the same finite element for the spatial discretisation. We choose $P1$ elements for both the vectorial space V and the scalar space Q, and we denote by V_h and Q_h respectively the finite element spaces.

The two finite dimensional spaces Q_h and V_h are originated from a (shape regular) mesh $\mathcal{T}_h$ with mesh size $h > 0$ for which we denote by $\mathcal{N}_h$ the set of vertices of the mesh. If we assume further that the meshes for the two domains coincide at the interface, we arrive at the following non-linear system of Differential Algebraic Equations (DAEs):

$$\begin{array}{ccccc} A_{TT}\boldsymbol{u}^T & A_{TS}\boldsymbol{u}^S & 0 & = & \boldsymbol{f}^T \\ A_{ST}\boldsymbol{u}^T & A_{SS}\boldsymbol{u}^S & -B^t p & = & \boldsymbol{f}^S \\ 0 & B\dot{\boldsymbol{u}}^S & C(\boldsymbol{u}^S)p & = & \boldsymbol{g}(\boldsymbol{u}^S) \end{array} \tag{15}$$

with $\boldsymbol{u}^T = \boldsymbol{u}^T(t)$, $\boldsymbol{u}^S = \boldsymbol{u}^S(t)$ and $p = p(t)$, $t \in (0,T_f]$. The matrices A, B, C are the representation operators on V_h and Q_h of the bilinear forms (14.1),(14.2),(14.3). Here, the superscript T refers to all nodes $x \in \mathcal{N}_h \cap \overline{\Omega^{\mathrm{Tooth}}} \setminus \overline{\Gamma^I}$ of the tooth domain Ω^{Tooth} which are not on the interface Γ_I and the superscript S to the vertices belonging to the the PDL domain Ω^{PDL} and to the interface Γ_I between the two domains.

For the discretisation of (15) in time we subdivide the time interval $I = [0,T_f]$ into K intervals of of constant time step size $\tau = T_f/K$ by means of the constant time step size $\tau > 0$. We set $t^j = \tau \cdot j$ and denote by $(\boldsymbol{u}^\alpha)^j$ the approximation of $(\boldsymbol{u}^\alpha)(t^j)$ at time t^j, $j = 0,1,2,\ldots,K$, where $\alpha \in \{S,T\}$. The same notation will be used for the pressure, as well.

Since, for stability reasons, an implicit discretisation is favourable for solving the non-linear Cauchy problem (15), we employ the following predictor-corrector scheme, cf. (Quarteroni et al. 2008): at each time step j we first compute the predictor $(\boldsymbol{u}^{j+1/2}, p^{j+1/2})$ according to

$$\begin{pmatrix} A_{TT} & A_{TS} & 0 \\ A_{ST} & A_{SS} & -B^t \\ 0 & B & \tau C((\boldsymbol{u}^S)^j) \end{pmatrix} \begin{pmatrix} (\boldsymbol{u}^T)^{j+1/2} \\ (\boldsymbol{u}^S)^{j+1/2} \\ p^{j+1/2} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f}^T \\ \boldsymbol{f}^S \\ \boldsymbol{g}((\boldsymbol{u}^S)^j) + B(\boldsymbol{u}^S)^j \end{pmatrix}.$$

Then, the following corrector step for determining $(\boldsymbol{u}^{j+1}, p^{j+1})$ is carried out

$$\begin{pmatrix} A_{TT} & A_{TS} & 0 \\ A_{ST} & A_{SS} & -B^t \\ 0 & B & \tau C((\boldsymbol{u}^S)^{j+1/2}) \end{pmatrix} \begin{pmatrix} (\boldsymbol{u}^T)^{j+1} \\ (\boldsymbol{u}^S)^{j+1} \\ p^{j+1} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f}^T \\ \boldsymbol{f}^S \\ \boldsymbol{g}((\boldsymbol{u}^S)^{j+1/2}) + B(\boldsymbol{u}^S)^j \end{pmatrix}.$$

As a consequence, in each time step we have to solve two linear systems of equations. For the solution of the both systems, we employ a Krylov space method (GMRES) in combination with a block diagonal Jacobi preconditioner. We note that also more elaborate techniques as multilevel preconditioners might be applied, see the work of Berrenberg and Krause (2007).

4. Experimental Studies and Validation

4.1 Setup of the In-vitro Measurements

We used a novel measurement set-up (see Figure 2) to determine the force-deflection characteristics of a porcine specimen. A piezoelectric actuator is used to apply displacements on the tooth's crowns via a thrust die. The point of displacement application is chosen in the centre of the labial side of the tooth's crown. Resulting forces are simultaneously recorded by an ultra miniature force sensor. Two cylindrical magnets are attached on the top of the tooth's crown. The movement of these magnets is detected using an array of eight Hall effect sensors for each magnet, and the movement of the loaded tooth is derived from the movement of the magnets.

The employed tooth in the present article is a premolar from a pig jaw bone segment. It was used for this investigation as the omnivore diet of pigs as well as the size (here, 21.5 mm height) of the pig's two-rooted premolars allow an easy transfer of the results to the human masticatory system.

As presented in the work of Berkowitz et al. (2009) the solid-fluid ratio is not uniform in the PDL and is in a range from 53% to 74%. Because it is not possible to know the effective distribution of the phases in the PDL we employ (see Table 1) a constant value $n_0^F = 0.4$.

We loaded the tooth by applying displacements of 0.16 mm with varying loading velocities. After experimentation we scanned the jaw bone segment in an in-house μ-CT scanner (SkyScan 1174, Belgium) and created a FE mesh of the relevant geometries (tooth and PDL) using the software ADOR3D (Rahimi et al. 2005). Figure 3 shows the resulting mesh which was used to validate our biphasic material model of the PDL by comparing the numerical results with the measured force-deflection behaviour of the same specimen, as described in the next sections.

4.2 Setup of the Numerical Simulations

The aim of our numerical simulations is the reproduction of the in-vitro measurements described in Section 4.1. In these experiments, time-dependent displacements are applied to the tooth and concurrently the force response on the tooth is measured. In Figure 4, a schematic representation of the two domains Ω^{Tooth} and Ω^{PDL}, and the subdivision of the boundary into Dirichlet and Neumann boundaries is shown. The simulations themselves were carried out employing the software toolboxes ObsLib++ (Krause 2007; Groß and Krause 2008) and UG (Bastian et al. 1997).

In these numerical simulations, the contact between the bolt and the tooth on $\Gamma_D^{\text{Tooth}} = \Gamma_D \cap \partial\Omega^{\text{Tooth}}$ is modelled by the following Dirichlet boundary condition

$$u(\boldsymbol{x}, t) = \frac{t}{T_f} u_{\max} \text{ on } \Gamma_D^{\text{Tooth}}$$

where in this case $u_{\max} = 0.16$ mm represents the maximum displacement reached in the normal direction x.

As described in Section 4.1, in the in-vitro experiments the force response of the system is measured by on the surface Γ_D^{Tooth} at the position of the bolt. Thus, in order to investigate the influence of the material parameters (cf., Section 4.3) we evaluate the boundary forces as follows

$$\int_{\Gamma_D^{\text{Tooth}}} \boldsymbol{T}(\boldsymbol{u})\boldsymbol{\nu} \cdot \boldsymbol{\nu} \, d\Gamma$$

Let us recall that for the in-vitro measurements we consider the system as composed by the tooth, the surrounding PDL, and the jaw bone. In the present investigation we consider short-time experiments so that orthodontic movements of the jaw bone do not occur. Therefore, on the external surface Γ_D^{PDL} (see Figure 4), where the PDL is in contact with the jaw bone, we apply Dirichlet boundary condition imposing a null displacement.

Finally, on all the remaining boundaries $\Gamma_N = \partial\Omega \setminus (\Gamma_D^{\text{Tooth}} \cup \Gamma_D^{\text{PDL}})$ we prescribe homogeneous boundary conditions. In our studies, we furthermore neglect the flow of the interstitial fluid through the surface between the PDL and the bone. Therefore, in Equations (9) and (14) we choose $f = 0$.

The objective of the next section is to study the influence of the parameters κ and k_0^F on the resulting displacement-force curve. All other parameters employed in the numerical simulations are reported in Table 1.

4.3 Study of Parameters: Towards a Validation of the Model

In this section we will employ the model presented in the previous sections to study the stress evolution under incremental loading. In particular, we study the influence of the zero displacement permeability k_0^F and the power κ on the forces in the tooth. Furthermore, we compare the obtained numerical results with those obtained from the in-vitro measurements. In these experiments the maximum displacement $u_{\max}$ is reached after 0.8 s, 2.0 s, and 4.0 s, respectively.

We remark that in case of deformations over 0.16 mm the stress curve shows an increasingly non-linear behaviour. Therefore, if large displacements above this value are prescribed, non-linear material laws should be employed in order to model the behaviour of the PDL.

4.3.1 Influence of the power κ

To show the influence of κ we focus on $T_f = 0.8$ second experiments where we choose different initial permeabilities for each κ : $k_0^F = 1 \times 10^{-6}$ m·s^{-1}, 1×10^{-7} m·s^{-1}, 1×10^{-8} m·s^{-1}. The results are shown in Figure 6.

As can be expected from the power law (5), larger choices of κ have increasing impact on the force-time curve, as can be seen in Figure 5. On the other hand, small choices of κ, e.g., $\kappa \in [1.0, 20.0]$, yield a sequence of very similar curves and will here be represented by $\kappa = 20$.

For initial, small deformations, a varying κ has almost no effect. But, after 0.3 seconds of our numerical simulations, the displacements become large enough such that $k^F(n^F) > 1$ and different choices of κ yield different force-time curves. But, as can be seen in Figure 5, increasingly larger choices of κ yield higher final stresses at T_f but do not change the shapes of the stress curves.

Let us remark that in the simulations, beginning from $\kappa \geq 38.0$, stress oscillations (see Figure 5(b)) occur which are due to the fact that the values in the matrix C in equation (15) become smaller.

4.3.2 Influence of the zero displacement permeability k_0^F and the final time T_f

The choice of the zero-displacement permeability is relevant both as initial force response and as long-term response. In Figures 6(a) and 6(b), we can see how the choice of k_0^F within equation (5) affects the behaviour of the stress-time curve. As can be seen in these plots, small values for k_0^F yield larger forces and vice-versa. In fact, since the initial permeability is a multiplicative constant within the operator C in (15), its influence should be comparable with choosing different time scales in the in-vitro measurements (Figure 6(c)).

The choice of a very small k_0^F, i.e., $k_0^F = 1 \times 10^{-8}$ m·s^{-8} yields forces that are very similar to the measured ones. On the other hand, the influence of such a small k_0^F is a significant change in the initial response of the system, in particular, we obtain larger stresses. Moreover, for small initial permeabilities, the shape of the time-stress curve significantly changes in comparison to larger choices of k_0^F, as can be seen in Figure 6(b).

4.3.3 A Comment on a Final Parameter Choice

Within the presented, different simulations, we employed different choices for the parameters in the Mow power law (5). As it turns out, the parameters that seem to give the best accordance between the numerical results and the in-vitro measurements are $\kappa \approx 35$ and $k_0^F \approx 1 \times 10^{-8}$ m·s^{-1}. In Figure 7, we compare the in-vitro measurements with numerically computed results where employing the above reported parameters but different final computation times T_f. However, a more precise data fitting would be too specific and would mask the behaviour of the model. Finally in Figure 8 we report the evolution of the normal stresses and of the pressure in two different time steps. In particular we can note increasing values of the normal stresses in the contact area with the bolt but with different sign in the superior and inferior part. High changes in the pressure are observed in the buccal side of the PDL. In Figure 9 we can see how in the areas of high pressure the fluid ratio decreases over time while the high fluid concentration in the upper part of the labial side can be noticed.

5. Conclusions

In this article, we considered a coupled biphasic-elastic material model for the simulation of a tooth-PDL system. A spatial and temporal discretisation with linear finite elements of the coupled system was presented.

The geometry employed in the numerical simulations results from a μ-CT scan of the same porcine tooth which was employed for the in-vitro measurement. Moreover, using our model, we were able to numerically reproduce the in-vitro experimental setup and obtain comparable stress-time curves. In this work, we were able to estimate a suitable range of parameters for Mow's power law. In fact, the model produces reasonable accordance for the resulting range of forces.

Further investigations are necessary since, in fact, our in-vitro measurements

but also the results in e.g, (Durkee 1996; Toms et al. 2002; Komatsu 2010) seem to reveal a viscoelastic behaviour of the tooth-PDL system. In particular, we observe a delay in the response to the initial displacements and a plateau at the end of the measurements. Therefore, in the focus of future investigations stands the extension of the biphasic material model by employing non-linear, anisotropic and viscoelastic material laws.

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Parameter	value	units
E_S	0.2e6	N m^{-2}
ν_S	0.3	#
E_T	20e9	N m^{-2}
ν_T	0.31	#
ρ^{RS}	$1,060$	kg m^{-3}
ρ^{RF}	$1,000$	kg m^{-3}
ρ^{T}	6,000	kg m^{-3}
n_0^S	0.6	#
n_0^F	0.4	#

Table 1.: Physical parameters in (3) used in the numerical experiments

Figure 1.: At each material point the two phases coexist and result in two different deformations $\boldsymbol{\varphi}^S$ and $\boldsymbol{\varphi}^F$.

Figure 2.: Measurement setup used for the in-vitro measurements.

(a) Labial side *(b)* Buccal side

Figure 3.: Geometries used for the simulations of the tooth-PDL system. In Figure (a) the labial side is shown and the contact area between the tooth and the bolt is highlighted. The contact surface is centred and 19 mm away from the root.

Figure 4.: Section of the employed domains: Ω^{Tooth} is the tooth domain and Ω^{PDL} denotes the PDL domain. The black line marks Γ_I, the interface between Ω^{PDL} and Ω^{Tooth}. Furthermore the regions where Dirichlet values are applied are marked by Γ_D^{Tooth} and by Γ_D^{PDL}.

(a) $k_0^F = 1 \times 10^{-6}$ m·s^{-1} *(b)* $k_0^F = 1 \times 10^{-7}$ m·s^{-1} *(c)* $k_0^F = 1 \times 10^{-8}$ m·s^{-1}

Figure 5.: Comparison of the influence of κ on the stress-time curves with different initial permeabilities k_0^F.

(a) $\kappa = 30$ *(b)* $\kappa = 30$ *(c)* In-vitro measurement

Figure 6.: The influence of small (a) and large (b) changes in k_0^F. In (c) the in-vitro measurements with different T_f are reported: the influence of small k_0^F has the same effect as accelerated in-vitro experiments.

Figure 7.: Comparison between measured force responses and simulated force responses for different T_f. Here we chose the parameters, as described in Section 4.3.3.

(a) Front side after 2 s *(b)* Back side after 2 s

(c) Front side after 4 s *(d)* Back side after 4 s

Figure 8.: Temporal evolution of the normal stresses in the tooth and of the pressure in the PDL.

(a) Front side after 0.7 s *(b)* Front side after 1.3 s *(c)* Front side after 2 s

(d) Back side after 0.7 s *(e)* Back side after 1.3 s *(f)* Back side after 2 s

Figure 9.: Temporal evolution of the fluid ratio in the PDL.