Data for: Establishment of a Numerical Model to Design an Electro-Stimulating System for a Porcine Mandibular Critical Size Defect

This repository contains geometry files for the creation of a model of an electrically stimulated minipig mandible and the corresponding finite element models.

General Information

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Objective

Modelling and simulation of electrical bone stimulation in a finite element model of a minipig lower jaw (mandible).

Problem Statement

In order to develop electro-stimulating implants for regeneration of bone defects, numerical simulations are an inevitable tool in the design process. We use finite element simulations to optimise the electrode configuration of an electro-stimulating implant for large defects in a minipig lower jaw.

Description

This data set provides the necessary computer-aided design project files (Materialise 3-matic) and 3D geometries to create the finite element model of an electrically stimulated minipig mandible that are described in the paper "Establishment of a Numerical Model to Design an Electro-Stimulating System for a Porcine Mandibular Critical Size Defect" published in the special Issue "Biomaterials for Bone Tissue Engineering" of the MDPI journal Applied Sciences (ISSN 2076-3417). Further, the finite element simulation models (COMSOL Multiphysics) are provided. The simulations allow to determine the electric field distribution and optimised stimulation parameters in the 3D model of the electrically stimulated minipig mandible.

Workflow

Firstly, CT data of a 17 month old male Göttingen minipig were segmented within the software Materialise Mimics version 19 (CT data and Mimics project files not included in this data set). The resulting 3D geometries of the minipig mandible and surrounding soft tissue were then further processed in the computer-aided design software Materialise 3-matic (*.mxp* files included in this data set) and STL geometry objects were created. The latter were imported into the finite element simulation software COMSOL Multiphysics version 5.4, where they were further manipulated and combined with geometric features.

Software involved (license needed)

- COMSOL Multiphysics version 5.4 (RRID:SCR_014767)
- Materialise Mimics version 19 (RRID:SCR_012153)
- Materialise 3-matic version 11

Description of files

Note that in order to create a geometry that can be properly imported to and worked with in COMSOL Multiphysics, many modelling steps had to be taken. These resulted in a variety of artefacts in terms of geometry files (*.stl*), COMSOL project files (*.mph*), and COMSOL geometry files (*.mphbin*). The import of the complete model geometry (*Minipig_complete_COMSOL.stl*) that has been exported from COMSOL, might work in other simulation software. However, it has not been tested so far, so we would recommend using the COMSOL geometry file *Weich_Kort_Spong_DifferenzDefektdif2.mphbin* together with COMSOL Multiphysics. Further information on how additional parts of the simulated geometry (implant, implant-tissue interface, boundary conditions, materials) were modelled, can be found in [1].

Files for creating the bone geometry

Minipig_Mandible.mxp Materialise 3-matic project in which the mandible geometry was imported that resulted from CT data segmentation in Materialise Mimics. The mandible geometry was further processed by repairing and smoothing the geometry.

Kortikalis_lochfrei_smooth.stl stl geometry file of the minipig mandible that resulted from the processing in *Minipig_Mandible.mxp*

Files for creating the complete head geometry with bone, soft tissue, and skin

SoftTissue_skin_bone.mxp Materialise 3-matic project in which the soft tissue domain was imported that resulted from CT data segmentation. Further, unnecessary parts of the geometry were removed (upper jaw, ears), the geometry was repaired and smoothed and uniformly remeshed. Additionally, a 2.28mm thick layer was added to mimic the skin. The mandible geometry *Kortikalis_lochfrei_smooth.stl* was imported, combined with the residual geometry into a non-manifold assembly. The resulting geometry object was finally exported as *SoftTissue_RG 17_smoothed_skin_cort.stl*.

SoftTissue_RG 17_smoothed_skin_cort.stl stl geometry file of the minipig head (i.e., mandible, surrounding soft tissue, and skin) that resulted from the processing in *SoftTissue_skin_bone.mxp*.

mphbin_ImportMitSpong.mph COMSOL Multiphysics project in which a generic geometry mimicking the cancellous (spongy) bone was created (basically out of an extruded ellipse). The resulting geometry was exported as *Spongiosa_ell.mphbin*.

Spongiosa_ell.mphbin COMSOL geometry object of the cancellous bone created in *mphbin_ImportMitSpong.mph*.

Spongiosa.mph COMSOL Multiphysics project in which Spongiosa_ell.mphbin was reimported and simplified via so-called *virtual operations*. The resulting geometry was exported as *Spongiosa_ell_virtOp.mphbin*.

Spongiosa_ell_virtOp.mphbin COMSOL geometry object of the simplified cancellous bone created in *Spongiosa.mph*.

Weich_Kort_Spong_DifferenzDefekt.mph COMSOL Multiphysics project in which the minipig head geometry (*SoftTissue_RG 17_smoothed_skin_cort.stl*) and the cancellous bone geometry (*Spongiosa_ell_virtOp.mphbin*) were imported. Further, the Boolean difference of head and cancellous bone was built. The resulting geometry object was exported as *Weich_Kort_Spong_DifferenzDefekt.mphbin*.

Weich_Kort_Spong_DifferenzDefekt.mphbin COMSOL geometry object of the minipig head with subtracted cancellous bone created in

Weich_Kort_Spong_DifferenzDefekt.mph.

Weich_Kort_Spong_DifferenzDefektgefüllt.mph COMSOL Multiphysics project in which *Weich_Kort_Spong_DifferenzDefekt.mphbin and Spongiosa_ell_virtOp.mphbin* have been reimported. The resulting final model geometry was exported as *Weich_Kort_Spong_DifferenzDefektdif2.mphbin.*

Weich_Kort_Spong_DifferenzDefektdif2.mphbin COMSOL geometry object of the final minipig head geometry including cancellous bone. Please note that some further geometric operations were performed inside the COMSOL simulation models (*Mesh_Convergence.mph*, *h_el_parametric.mph*, *Optimise_Pot.mph*) themselves.

Minipig_complete_COMSOL.stl stl geometry file of the complete minipig model that has been exported from COMSOL Multiphysics in order to enable also readers without COMSOL access to view and work with the final model geometry. However, please note that during the export in COMSOL the geometry has been slightly deformed.

To reproduce the simulation results it is recommended to use the COMSOL geometry file *Weich_Kort_Spong_DifferenzDefektdif2.mphbin.*

Simulation models

Please note, that the simulation models were saved without solutions in order to avoid huge file size. Hence, the studies need to be recomputed in order to reproduce the results.

Mesh_Convergence.mph COMSOL Multiphysics model to study the mesh convergence behaviour of the finite element model. However, prior to simulation some further geometric operations were performed inside the geometry module of COMSOL. This includes creating, moving, and subtracting a block from the geometry in order to model the bone defect. Further, the model geometry was complemented with the electro-stimulating implant that resulted from extrusion of a circle in a work plane parallel to the defect boundary. Finally, *virtual operations* were used to simplify the geometry and accelerate the computations. Details on the assigned material, physics, boundary conditions, and study settings can be viewed in [1]. The chosen implant parameters for this study were a stimulation amplitude of 1V and a electrode length of 20mm. The mesh convergence included changing the mesh parameters (maxel, minel, elgro, curv, res) in a parametric sweep (study3). For each mesh configuration, the total electric energy in the whole computational domain was computed. Computing the relative error of the electric energy with regard to the finest mesh, a mesh configuration with relative error below 0.04% (Mesh 2 Chosen, study4) was chosen for the following simulations studies in h_el_parametric.mph and Optimise_Pot.mph.

h_el_parametric.mph COMSOL Multiphysics model to study the impact of changing the electrode length (parameter h_el) in order to achieve a maximum volume of beneficially stimulated tissue in the defect domain. A stimulation amplitude of 1V was applied. Via volume integration, the volume of beneficially stimulated, understimulated, and overstimulated tissue in the defect domain has been determined for each parameter value of h_el.

Optimise_Pot.mph COMSOL Multiphysics model to optimise the applied stimulation voltage (parameter PotStim). The optimal electrode length of 25mm resulting from h_el_parametric.mph was used in this study. In the *Optimization* interface, Integral Objective Functions for beneficial stimulation, understimulation, and overstimulation were defined (for further details see [1]). PotStim was varied between 0.2V and 4V and the Nelder-Mead method was used to determine the optimal stimulation potential (study1). Further, using the optimal stimulation parameters, the conductivity of the defect domain was varied parametrically in study 2.

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Bibliography

[1] Hendrikje Raben, Peer W. Kämmerer, Rainer Bader, Ursula van Rienen. Establishment of a Numerical Model to Design an Electro-Stimulating System for a Porcine Mandibular Critical Size Defect. *Applied Sciences* 9, 2019.