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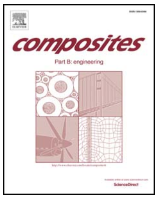

Multi-scale modelling and simulation of a highly deformable embedded biomedical textile mesh composite

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ABSTRACT

Self-healing prostheses that can replace damaged native organs, like tissue-engineered valvular implants, are under development. Engineered soft tissues can greatly benefit from reinforcements to attain mechanical properties comparable with the native organs. Complex interactions at various levels between the reinforcements and engineered tissue make the selection of the most optimized reinforcing scaffold difficult and subject to an enormous amount of experimental evaluation. Hence, to reduce the extent of prototyping, it is prudent to develop a simulation based development approach. In the example of valvular prostheses which are textile-tissue composites, we test a simulation approach based on multi-scale modelling, often used for evaluating/predicting the behaviour of composites. A textile scaffold embedded in silicone is used as a replacement for the textile-tissue composite. The modelling technique provides a good correlation with the experimental results, laying the pathway to further study the complex interaction between the engineered tissue and the reinforcing scaffold. This method can further form the basis for evaluating the mechanical compatibility of scaffolds and their interaction with engineered tissues at various scales and levels.

1. Introduction

Engineered biomaterials are ubiquitous and have important function in numerous biomedical applications. One such application of biomaterial implants is tissue-engineered heart valves for surgical or transcatheter implantation [1,2], where replacement of self-healing, load-bearing soft tissues is an impetus for their development. In most cases, pure engineered tissues do not possess the mechanical properties required by such implants to sustain the working pressures of the systemic circulation. This can be overcome with the use of reinforcing scaffolds. An optimum scaffold architecture for tissue-engineered heart valves is a structure with a high degree of interconnectivity (through continuous or interconnected short fibres) allowing for uninterrupted stress flow through the thin heart valve leaflets to the strong aortic wall, protecting the cusps from rupture yet being porous enough to allow cellular in-growth. In the current work, a textile mesh (knitted scaffolds) used in the development of tissue-engineered tubular aortic heart valves [1,3] has been used as an example.

Currently, the reinforcing scaffold is intuitively chosen without any prior mechanical compatibility evaluation in terms of meso- and micro-mechanisms of deformation. This is because it is complicated to formulate a quantitative criterion as not only are the values often missing, but even the quantities to be evaluated are not clearly defined. Therefore, characterization should be performed at the macro- and microscopic length scales (multi-scale properties) because a mismatch between highly deformable engineered tissue and scaffolds can lead to short and long-term health impairments. Hence, the mechanical compatibility of reinforcing scaffolds depends not only on the properties and composition of the material, but also on its organization, distribution and motion at one or several length scales. Various biocompatible scaffold heart valves were tested by Van Lieshout et al. [4,5] under systemic circulation, concluding that the knitted scaffolds lasted longer compared to their electro-spun counterpart.

In their review, Mazza and Ehret [6] elaborated that mechanical compatibility of highly deformable reinforcing scaffolds depends more on their deformation behaviour rather than on their strength. In fact, integration of engineered tissues with textile mesh are not only associated with adequate macroscopic properties (non-linear stress strain response, ductility, strength) but also with their realization by micro-structural kinematics which should match those of the adjacent tissue. Mechanical interaction is determined by the spatial arrangement i.e., the topology of the micro-structure, governing the local and global

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deformation behaviour. Length scales responsible for the mechanical response depend on the material system and are in the range of mm for such prosthetic meshes. Multiple measurements for different loading states are required to reliably characterize the deformation behaviour of such scaffolds. Therefore, to achieve design and mechanical compatibility, modelling strategies to rationalize experimental observations and predict implant performance need to be developed.

There are three major modelling approaches of textile fabrics, namely continuum, structural and multi-scale methods. Significant amount of work in representing the continuum macroscopic behaviour of differently oriented fibre reinforced material has been developed in the last few decades. Much of the works on continuum modelling of isotropic and anisotropic material behaviour has been reviewed in Chagnon et al. [7]. The continuum macro-scale approach like the ones proposed in Hernández-Gascón et al. [8] and Yeoman et al. [9] can be easily implemented into FEM code to efficiently simulate inhomogeneous load cases which is not straight forward in other meso- or micro-scale methods. However, fabrics are not a continuum and a large experimental data set is needed to fit the corresponding model parameters.

The central idea behind the structural models is to use a physically motivated meso-scale structure to capture the relevant mechanical phenomena at the macro-scale. In this way suitable criteria for fabric design and optimization can be deduced. Weaves are the simplest structure among fabrics and are the most examined in the literature, see Refs. [10–16]. These structural models focus primarily on yarn-yarn interaction such as shear-locking or crimp interchange in tension. Macro-scale phenomena simulated by such models include geometric non-linearity, non-linear force-strain relationships, large Poisson's ratios or anisotropy. There are only a few structural models for knitted textiles, e.g. Antonietti et al. [17] and Röhrnbauer et al. [18]. A repeating unit cell (RUC) of knitted prosthetic mesh based on the theory of multi-body systems showing good correlation with effective macro-scale experimental results and local non-affine deformation state was proposed by Röhrnbauer et al. [18]. However, as these models generally use truss or rigid force elements and the presence of matrix is usually either implemented as boundary conditions or enforced in model equations, it is not possible to extract the local stress and strain fields in the matrix. These values are important to determine the growth and remodelling of tissues. Also, since the method is physically motivated, large number of parameters are needed to account for stitches, nodes or cross-links.

An equally popular method is the use of detailed micro-scale approach, see Refs. [19–21]. Due to their complex inter-looping patterns, knitted dry fabrics are more frequently modelled at the micro-scale with an explicit representation of each filament/yarn [19–21]. A review of such modelling approaches can be found in Hasani et al. [22], Huang and Ramakrishna [23], Tan et al. [24] and Hallal et al. [25]. The geometries and assigned material properties for the filaments/yarns are based on real measured data. Therefore, such detailed models are associated with lesser model assumptions. Virtual experiments with perfectly controlled boundary conditions can be performed on such models. Three-dimensional micro-structural effects, which cannot be evaluated with other models and are generally difficult to be seen from experiments, can be examined through finite element analysis. However, such models are often computationally expensive and require the solution of multi-contact problems, which often lack numerical convergence or require non-physical assumptions on the friction behaviour and the inter-penetration of filaments [19]. Another challenge is the definition of a representative initial configuration, which might be found by an elaborate simulation of the manufacturing process and the corresponding solution of the unloaded equilibrium state, see Refs. [21,26].

Multi-scale modelling of knitted fabrics with basic looping structures are presented in Wan et al. [27]. Multi-scale approaches are also aimed at determining parameters for corresponding constitutive model formulations to be implemented in finite element codes. There has been tremendous development in the field of multi-scale material modelling of traditional fibre reinforced composites, investigating the effects of micro structure on its macroscopic behaviour. Nguyen et al. [28] reviewed the recent developments in multi-scale modelling of continuous and discontinuous multi-phase heterogeneous materials. Vassiliadis et al. [29] discussed the challenges and solutions for modelling methodologies of woven fabrics at different scales accounting for micro to macro-scale deformations. An extended literature review of the computational models for the deformation of woven fabrics was presented. A review on homogenization and topology optimization of periodic structure was presented by Hassani and Hinton [30] and Saeb et al. [31].

Geometric modelling approaches for different fabrics and its composites have been presented in literature [32–37]. A representative volume element (RVE) based approach to determine the effective stiffness of a multi-layered biaxial weft-knitted fabric reinforced composite was presented in Qi et al. [38]. Ugbolue [39] examined the geometrical model of auxetic warp knit structures and validated their characteristics with data obtained from experimental analysis.

Even though there is a considerable body of work in various disciplines like modelling of biomaterials, analysis of dry scaffolds and multi-scale modelling of fibre reinforced composites, there is a scarcity in the synergistic approach in determining the mechanical compatibility of scaffolds used in implants. The present work is devoted to a multi-scale method for modelling, simulation and analysis of textile composites used in the development of a tissue-engineered tubular aortic heart valve. In-silico experiments are conducted at various structural levels to predict the macro-scale mechanical behaviour of the textile composite and quantify the local deformation kinematics. A hierarchical multi-scale modelling approach popular in the field of material mechanics is employed. The benefit of this approach is that individual constituents of the composite can be modelled by means of a simple material model, and characterized using standard experiments.

2. Experiments

In the present work, a textile-silicone composite was used for validation of the proposed numerical methods. This is because, once the textile is embedded in a tissue matrix, it's mechanical behaviour changes as the deformation mechanics are modified by the ingrowth of tissues. And, in Röhrnbauer and Mazza [40] and Röhrnbauer et al. [18], it was shown that when a textile scaffold is embedded into elastomer matrix, its results have the same qualitative conclusion when compared to the corresponding experiment on ex-plants (i.e. dry textile mesh surrounded/embedded into tissue). Also, in contrast to textile-tissue, textile-elastomer composites are easy to handle and inexpensive with test results showing moderate scatter, establishing themselves as an effective tool for mechanical characterization/optimization and validation of numerical methods & models for prosthetic meshes preceding in-animal study. Another advantage of using a textile-elastomer composite as a model for tissue in-growth is the quantification of non-affine deformation mechanisms and local delaminations [41].

2.1. Textile-silicone composite

The textile mesh was produced using medical grade polyethylene terephthalate (PET) fibres. For the production, a tüll-fillet pattern, a needle gauge of E30 (i.e. 30 needles per inch) and a course density of 15 loops/cm were chosen. 52 PET yarns were processed into a tubular structure which was thermo-stabilized at 200°C for 8 min before use. The textile mesh was then embedded into a medical grade silicone matrix and cured for 2 h. A specimen is shown as an insert in Fig. 1 and dimensions of the produced specimens are provided in Table 1.

The tensile test set-up, which included a Zwick Z005 testing machine along with a specimen is shown in Fig. 1a. The specimens were