Computational investigation of the impact of assumption of affine deformation on constitutive models of soft tissues

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Abstract

All constitutive models proposed during the last decades for large strain composites with hyperelastic matrix use an intrinsic assumption of affine deformation between the matrix and reinforcing fibres. While for typical technical composites the affinity of deformation between fibres and matrix till high loads is ensured by targeted creation of their chemical bonds, this need not to be the case with soft biological tissues. For instance, this assumption might be disputable for arterial tissues with their matrix consisting of very compliant gel-like proteoglycans. On the other hand, no constitutive model proposed till now has been capable to give a reasonable fit of all mechanical tests of some pathological tissues with low initial stiffness, such as aortic aneurysm wall. Thus, a question occurs whether this discrepancy could not be caused by the intrinsic assumption of affine deformation used in all models. To test the impact of this assumption on the simulated response in some mechanical tests, two finite element models of specimens of arterial tissues were created, both including matrix and fibres separately. The former model mimicked the affine deformation of matrix and fibres by merging all the nodes of both components, while the deformation of fibres was independent of the matrix in the latter model, with exception of both fibre ends. Differences in reaction forces of specimens were evaluated in various strain states and directions with respect to the orientation of fibres. The evaluated differences between models with affine and non-affine deformations were significant but smaller than typical inaccuracies of constitutive models when fitting aortic aneurysm tissues.
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Keywords: fibre composite, hyperelastic matrix, finite element analyses, affine deformation, soft tissue

1. Introduction

Computational modelling becomes an important tool in all engineering analyses. While applicability of analytical calculations is rather limited in the field of non-linear (large displacements and large strain) mechanics, since the last decade of the 20th century finite element method (FEM) has enabled analyses of general bodies of materials showing large strains, both plastic and elastic. For large strain elasticity, the hyperelastic approach is mostly applied, based on postulating a strain energy density function. Thus a number of isotropic constitutive models have been proposed in the 20th century (e.g. Mooney-Rivlin model [16, 21] and its simplified forms such as Yeoh [29], Arruda-Boyce [1], Ogden [17], etc.). These models have been applied not only for technical elastomers like rubber but also for description of soft biological tissues, and nowadays constitutive models represent a challenging and important issue in biomechanics. Although in some simple cases stresses in arterial wall may not depend significantly on its properties, its constitutive models become relevant in more complex shapes (aortic aneurysms, arterial bifurcations, arteries with atheroma, etc.) or due to structural non-homogeneity of the wall. The importance of constitutive models for prediction of stresses in aneurysm wall was

analysed in [13] and advantages of structure based models in [18]. In this field some new models have been also proposed, both isotropic such as Demiray [5] and anisotropic such as Fung [4], Hayashi [25], etc. These anisotropic models are purely phenomenological which may appear limiting when a good predictive capability of the model is required. As biaxial tension is typical for arteries in vivo, inflation tests of tubular specimens are preferred because they mimic the physiological state of stress in arterial wall very closely. If tubular specimens are not disposable, biaxial tension testing of square shaped specimens may be an option; if tested under different displacement or force ratios between both loading directions, the responses can also cover all the physiological stress-strain states of the artery. However, often the artery specimen size enables uniaxial tension testing only (typical for small or diseased arteries). Then the predictive capability, specifically a correct description of tissue behaviour under biaxial tension on the basis of uniaxial tension tests, represents a highly important quality of a constitutive model [24]. Validation of the models is mostly done by means of comparison of model prediction with results of different (uniaxial as well as biaxial) tension tests.

Structure based models reflecting the tissue structure at different levels (e.g. Lanir [11], Holzapfel [8], Gasser [7], Martufi [14]) were expected to have better predictive capabilities than the above mentioned phenomenological models [24]. Many of these models are capable to describe uniaxial or biaxial passive response of arterial tissues with acceptable accuracy but most of them fail in prediction of biaxial response on the basis of uniaxial testing only. A similar problem occurs if stress-strain behaviour of arterial tissue under various types of biaxial stress or strain is to be predicted based on equibiaxial tests only. Therefore, biaxial testing under different ratios of displacements, forces, or strains in both directions has been introduced and preferred. However, some contradictions occurred when evaluating data related e.g. to abdominal aortic aneurysm (AAA) wall. The models fitted to uniaxial tests showed several times higher initial stiffness than those fitted to different biaxial testing data; this effect was found when comparing number of different studies [19, 20, 26, 27]. Moreover, some unpublished data measured in our lab with AAA wall showed similar discrepancies; for instance, when we tried to capture the experimental responses measured with the same specimen under four different force-controlled biaxial loading protocols, none of known constitutive models, including several anisotropic structure based ones, was capable to describe them reasonably. For this purpose, we used Hyperfit software (http://www.hyperfit.wz.cz) offering much better options than any commercial FEM software. Nevertheless, most of the models intended for arterial tissues gave negative coefficient of determination R^2, with exception of some variants of Mooney-Rivlin and Ogden models which, however, reached $R^2 < 0.5$ only. To explain these discrepancies, we hypothesized (in [24]) it might be due to non-affine deformation of fibres and matrix in the tissue which would contradict the intrinsic assumption of all structure-based models. Also, some other published results [2, 10, 15] support this hypothesis on importance of affine deformation.

Although the impact of constitutive models on stresses in arterial tissues, especially in AAAs, is frequently investigated in literature (see e.g. [9, 13, 18] and references therein) the problem of affine deformation has been seldom addressed. While for typical technical hyperelastic composites (e.g. rubber reinforced by textile or steel fibres as used in some parts of car tyres) the affinity of deformation between fibres and matrix till high loads is ensured by targeted creation of their chemical bonds, this need not to be the case with soft biological tissues. In [3] the authors show theoretically that in the case of tissue equivalents based on hydrated networks of collagen fibrils the affine deformation cannot be expected. The fibre stresses under uniaxial tension calculated using this assumption were three times higher than using a model with a free deformation of the fibre network. A recent paper [10] shows experimentally that the assumption

of affine deformation may cause a severe under- or over-estimation of fibre reorientation in adventitial layer of carotid arteries in dependence on the state of stress and strain. In the submitted paper we analyse the impact of affine and non-affine deformation between the matrix and fibres in arterial tissue on global tissue response under uniaxial and biaxial extension by means of finite element (FE) simulations of the corresponding mechanical tests.

2. Materials and methods

For computational simulations we have used FE software package ANSYS 17.0 (ANSYS Inc. PA, USA); we have created FE models of a square-shaped specimen of a fictitious soft tissue with one family of collagen fibres oriented under variable angle to the direction of the dominant load. Although tubular specimens are often used in arterial testing to achieve states close to physiological ones, the square-shaped specimen also enables us to achieve a nearly homogeneous state of stress in the model under different types of biaxial stress. This shape is preferred when tubular specimens are not available (typically for human arteries, e.g. AAA wall). The matrix was represented by two layers of 2D (linear) shell elements parallel to the specimen middle plane, each with half thickness of the specimen. They are based on Mindlin shell theory thus they apply only one integration point throughout the thickness and linear distribution of displacements throughout the thickness is assumed. The fibres were modelled with similar shells oriented in the chosen fibre direction and perpendicular to the middle plane of the specimen (see Fig. 1); their thickness was set small enough to ensure their negligible bending stiffness, similar to collagen fibres. A mapped mesh was created manually; the shells representing infinitesimally thin fibres distributed uniformly throughout the specimen thickness were divided into multiple elements along the fibre length; for affine deformation, all these nodes were merged with the closest nodes of the upper and lower shell representing the matrix. In contrast, for non-affine deformation the displacements of nodes along the fibre length were independent of matrix with exception of their end nodes. Due to uniform distribution of stresses and strains throughout the specimen thickness, one shell element throughout the thickness was sufficient, thus the total number of elements was on the order of 10^3 only, with 10^2 of them representing the fibres; the number of degrees of freedom exceeded 10^4. Full Newton-Raphson integration scheme was used and simulation of one case took several minutes on a 6 CPU computer with 16 GB RAM.
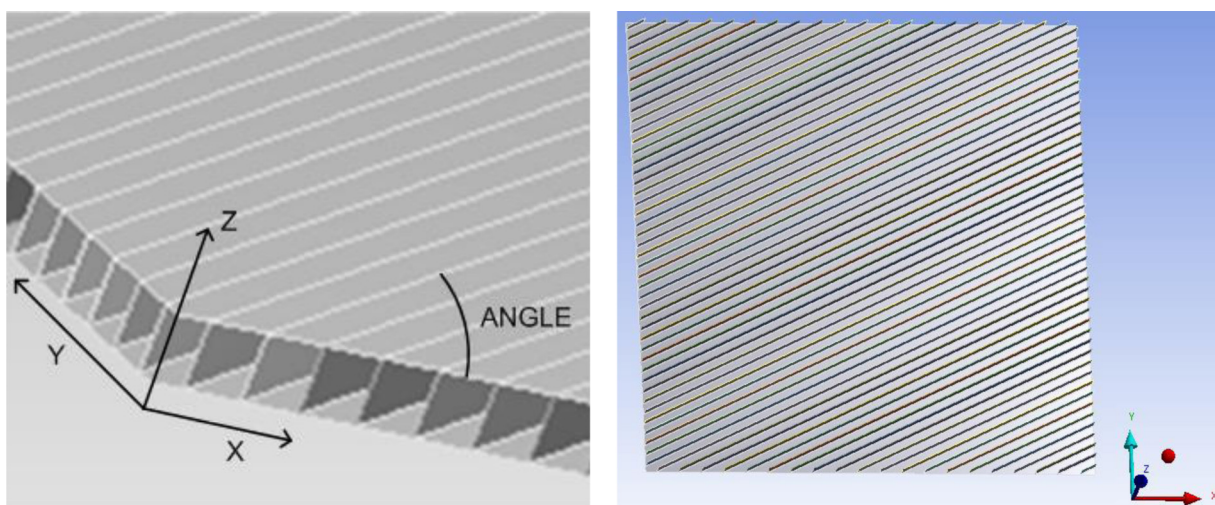

Fig. 1. Shell FE model of arterial tissue used in the simulations. The angle of fibres ($25°$ in the right figure) is defined with respect to X axis. Biaxial loading acts in X and Y directions

Material properties of the fibres correspond to wavy collagen fibres [28] and are described with 5-parameter Yeoh strain energy density function as follows:

$$\psi = \sum_{i=1}^{5} c_i (I_1 - 3)^i,$$

where I_1 is the first invariant of right Cauchy-Green deformation tensor and c_i are stress-like parameters of the model having the following values: $c_1 = 10\,\text{Pa}$, $c_2 = 8 \cdot 10^6\,\text{Pa}$, $c_3 = c_4 = 0$, $c_5 = 2 \cdot 10^8\,\text{Pa}$.

Mechanical behaviour of the matrix (corresponds to non-collagenous matrix of healthy arterial tissue) is described with Neo-Hookean hyperelastic constitutive model, given by the same strain energy density function and its parameters $c_{10} = 1 \cdot 10^4\,\text{Pa}$ (shear modulus of $20\,\text{kPa}$), $c_{20} = c_{30} = c_{40} = c_{50} = 0$. Both materials were modelled as incompressible. Uniaxial stress-strain curves of both components are depicted in Fig. 2.
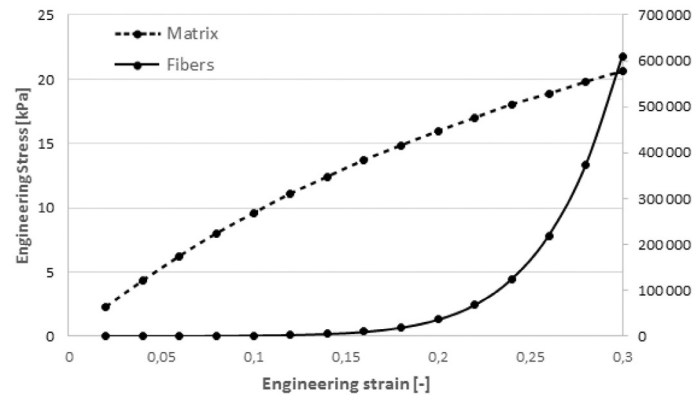

Fig. 2. Uniaxial stress-strain curves of the matrix (left scale) and the fibres (right scale)

The angle of fibres was changed from $0°$ up to $90°$ with a step of $5°$. Boundary conditions were prescribed to mimic different stress-strain states, i.e. uniaxial tension, plane strain tension (with transversal deformation restricted), both loaded in either X or Y direction, and five different biaxial stress states with strain ratios between both loaded directions of $1 : 5$, $1 : 2$, $1 : 1$ (equibiaxial), $2 : 1$, $5 : 1$. Strain in the dominantly loaded direction was set up to 30% while the transversal displacement-controlled load was proportionally reduced. Shear in-plane deformation of the specimen was restricted by application of symmetry conditions on some specimen edges.

Under the maximum load the reaction forces in both directions were evaluated, recalculated into engineering stresses in a standard way and compared between the corresponding models with affine and non-affine deformation. To calculate the relative (percentage) difference between affine and non-affine deformation, the stress calculated under assumption of affine deformation was taken as a basis.

3. Results

As expected, the shape of the fibres was curved for the affine and straight for the non-affine deformation. The differences between both models were highly angle-dependent and ranged up to 10 percent. They are presented for stresses in X direction and all the solved models in Fig. 3; for models loaded in y direction the results for α angle are identical with the corresponding
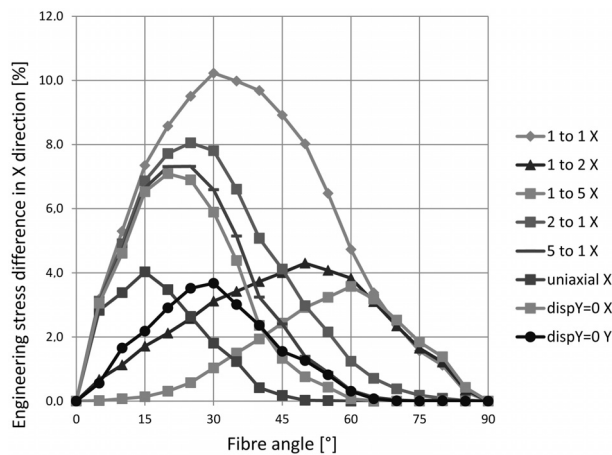
Fig. 3. Dependence of relative differences in stresses on the fibre angle. The type of loading protocol is defined by means of displacement ratio between both loading directions. "2 to 1 X" means dominant load in X direction with Y displacement being two times lower
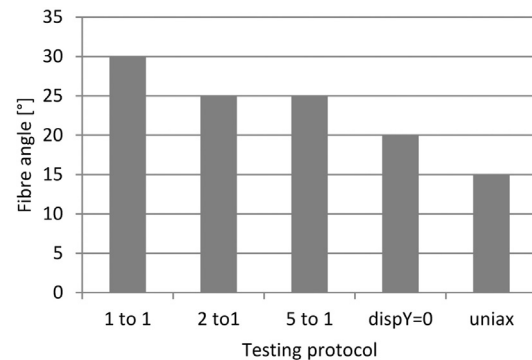
Fig. 4. Fibre angles with maximum relative differences for different stress-strain states

model with fibres oriented under $(1 - \alpha)$ angle and loaded in X direction. The impact of non-affine deformation depended strongly on the fibre direction; it was naturally zero for longitudinal or transversal orientation of the fibres and achieved its maximum for the fibre angles between $15°$ and $30°$. The position of this maximum changed with the type of stress-strain state similarly to the magnitude of this difference. Maximum difference was found under equibiaxial tension while it decreased with decreasing transversal displacement. This tendency was visible not only at proportional biaxial tests but also at planar tension (transversal deformation is zero) and at the uniaxial tension test (transversal deformation is negative). For all fibre angles the maximum difference occurred under equibiaxial tension.

The fibre angles with maximum difference are presented in Fig. 4. There is also an evident tendency of decreasing angle with maximum difference with decreasing transversal deformation, but it cannot be quantified more accurately due to the stepwise changes in fibre angles with the step of $5°$. For the states with dominant load in Y direction, the angle with maximum difference is higher than $45°$, i.e. the maximum difference occurs for the fibres oriented more longitudinally, closer to the direction of the dominant load.

4. Discussion

The applied FE element model represents a significant simplification of reality; the most remarkable one is application of shell elements. A more rigorous model with fibres created by means of volume elements with respecting their full 3D geometry is extremely large and time-consuming [12], and it was used only to confirm negligible differences of the applied shell model. Moreover, a full 3D model shows other limitations because the number of elements needed for both fibres and matrix increases with decreasing diameter of the fibres; and the fibre diameter is taken infinitesimal in the above mentioned structure based constitutive models. Application of tension only (denoted as LINK in ANSYS) or tension and bending (BEAM) elements would bring other difficulties in prescription of deformation being affine with the volume elements representing the matrix; moreover, they both do not support hyperelastic constitutive models in the actual version of ANSYS software. Therefore, the SHELL elements appeared as the best

choice as they represent infinitesimally thin fibres uniformly distributed throughout the specimen thickness and the shell thickness can be (and was) set to correspond to the real diameter of collagen fibres. As the SHELL elements have also some rotational degrees of freedom, their use also for the matrix was a natural choice to ensure an easy way how to prescribe affine (i.e. the same) deformation for both fibres and matrix.

The presented analysis was done only for one combination of materials of fibres and matrix, corresponding to healthy arterial tissue. Therefore, a quantitative impact of other material models is expected and the results cannot be generalized to significantly different materials. For the investigated type of soft tissue, however, the results show a significant impact of the assumption on affine deformation on the stress-strain response of the tissue. The maximum difference of 10%, however, cannot explain the discrepancy between experiments and the structure based model which we found for AAA tissues; negative R^2 obtained with all structure-based models represents a much higher discrepancy.

Also, unidirectional arrangement of fibres represents a certain limitation of our model, because controversial results exist concerning the number of fibre families in arterial tissues. Our comprehensive analysis has shown a dominantly uniaxial (circumferential) arrangement of collagen fibres in inner layers of porcine aortic wall with their dispersion increasing continuously to nearly isotropic distribution in the outermost layer [18]. Although many papers report on two fibre families in arterial tissues (e.g. [22] for rabbit arteries or [23] for human aortas and iliac arteries), we have shown that the preference of two fibre families is not well supported and specifically these experimental results correspond better to a unimodal distribution [6]. One family of dispersed fibres is very frequent in all types of arteries including humans and for such a distribution only the dispersion is neglected; it has only minor quantitative influence on the results, thus the unidirectional arrangement of fibres represents a reasonable simplification of this type of tissue and also an upper limit for impact of two symmetric families of fibres assumed by many constitutive models (e.g. [7, 8]).

The rare results published till now on affine deformation encouraged us to expect a more pronounced difference between affine and non-affine deformation of arterial tissue. A network model resulted in roughly threefold lower macroscopic stresses compared to the affine model [3]; however, that model related to interconnected network of fibres while our model contains separated fibres. Also the recently published contradiction of the affine model predictions with experimental results [10] cannot be explained with a continuous model and the authors offer an explanation on the basis of a tensegrity model of extracellular matrix. This might be also the reason why structure based constitutive models cannot offer a reasonable approximation of different types of biaxial tests with AAA tissues. Moreover, the problem may also consist in oversimplification of the macroscopicallyy homogeneous model of the arterial wall because different arterial layers show different structural arrangement of fibres. However, our own experiments were done only with a whole AAA wall because for pathological arteries the separation of individual layers becomes more difficult and it is hardly feasible for the AAA wall. Therefore, multilayer models remained out of scope of this study although they might bring better results; they should be investigated in future.

5. Conclusion

On the basis of the realized FE simulations of different types of uniaxial and biaxial tension tests it can be concluded that the assumption on affine deformation of fibres and matrix, being intrinsic for all structure based models of arterial tissues, may have a significant impact on the calculated stresses. However, quantitatively this impact has not exceeded 10% and cannot

explain the fact that structure based models, similarly to most of the phenomenological ones, give extremely low, even negative R^2 when fitting multiple biaxial tests of AAA wall and thus fail completely in description of experimental responses of such tissues. Evidently this problem is worth to be analysed in greater detail in future.

Acknowledgements

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