Porous Fibre-Reinforced Materials Under Large Deformations

Salvatore Federico
Department of Mechanical and Manufacturing Engineering, The University of Calgary
2500 University Drive NW, Calgary, Alberta, T2N 1N4, Canada
Phone: +1-403-220-5790; Facsimile: +1-403-282-8406; E-mail: salvatore.federico@ucalgary.ca

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SUMMARY. Soft biological tissues can be represented by a porous matrix saturated by a fluid and reinforced by a network of statistically oriented, impermeable collagen fibres. A homogenisation method has been developed for porous fibre-reinforced materials with an isotropic matrix, under small deformations [2], and its application to articular cartilage correctly predicted some specific aspects of the anisotropy and inhomogeneity of the permeability of the tissue [3]. The aim of this work is to generalise this model to the case of large deformations, and of matrix with an anisotropic permeability. The whole framework is set in general coordinates, with the employment of the material and spatial metric tensors.

1 THEORETICAL BACKGROUND

The Continuum Mechanics notation adopted here is almost identical to that in Marsden and Hughes [5]. With the exception of two-point tensors (an example of which is the deformation gradient $\boldsymbol{F}$), uppercase letters are reserved to material quantities, and lowercase letters to spatial quantities. In order to respect this customary use in modern Continuum Mechanics, a notation at times substantially different from that in [2, 3] has been adopted in the development of the theory.

1.1 *Basic Continuum Mechanics*

The deformation is described by the configuration χ, mapping *material* points $X = (X^1, X^2, X^3)$ in the reference configuration $\mathcal{B} \subseteq \mathbb{R}^3$ into *spatial* points $x = (x^1, x^2, x^3)$ in the natural Euclidean space $\mathcal{S} = \mathbb{R}^3$. At each point $X \in \mathcal{B}$, the two-point tensor $\boldsymbol{F}(X) : T_X\mathcal{B} \to T_x\mathcal{S}$ is the deformation gradient, mapping vectors in the tangent space $T_X\mathcal{B}$ at X into vectors in the tangent space $T_x\mathcal{S}$ at $x = \chi(X)$. $\boldsymbol{F}$ has components $F^i{}_I = \chi^i{}_{,I} = \partial\chi^i/\partial X^I$, and its determinant $J = \det\boldsymbol{F}$ is the volumetric deformation ratio.

The fully material tensor $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$, with components $C^I{}_K = g_{ij}F^j{}_J G^{JI} F^i{}_K$ is the right Cauchy-Green deformation tensor, with inverse $\boldsymbol{B} = \boldsymbol{C}^{-1} = \boldsymbol{F}^{-1}\boldsymbol{F}^{-T}$. The fully spatial tensor $\boldsymbol{b} = \boldsymbol{F}\boldsymbol{F}^T$, with components $b^i{}_k = F^i{}_I g_{kj} F^j{}_J G^{JI}$ is the left Cauchy-Green deformation tensor, with inverse $\boldsymbol{c} = \boldsymbol{b}^{-1} = \boldsymbol{F}^{-T}\boldsymbol{F}^{-1}$.

The material identity tensor is $\boldsymbol{I}$, with components $I^I_J = \delta^I_J$. The material covariant metric tensor $\boldsymbol{G}$ has components G_{IJ}, and its inverse $\boldsymbol{G}^{-1}$, the material contravariant metric tensor, with components G^{IJ}, is denoted $\boldsymbol{G}^\sharp$. Tensors $\boldsymbol{G}$ and $\boldsymbol{G}^\sharp = \boldsymbol{G}^{-1}$, lower contravariant indices and rise covariant indices, respectively. For example, if $\boldsymbol{W}$ is a vector with (contravariant) components W^I, its associated covector is $\boldsymbol{W}^\flat$, with (covariant) components $W_I = G_{IJ}W^J$. Conversely, if $\boldsymbol{Q}$ is a covector with (covariant) components Q_I, its associated vector is $\boldsymbol{Q}^\sharp$, with (contravariant) components $Q^I = G^{IJ}Q_J$. The definitions of the spatial identity tensor $\boldsymbol{i}$, spatial covariant metric tensor $\boldsymbol{g}$, and spatial contravariant metric tensor $\boldsymbol{g}^\sharp = \boldsymbol{g}^{-1}$, as well as the use of the metric tensors to lower and rise indices, are analogous to the material case.

The *push-forward* and *pull-back* operations on contravariant and covariant quantities follow different rules, which can be summarised in the scheme below.

		contravariant	covariant
push-forward	$\chi_*[\,\cdot\,]$	$\boldsymbol{F}$	$\boldsymbol{F}^{-T}$
pull-back	$\chi^*[\,\cdot\,]$	$\boldsymbol{F}^{-1}$	$\boldsymbol{F}^{T}$

For example, the push-forward of the material vector $\boldsymbol{W}$ is the spatial vector $\boldsymbol{w} = \chi_*[\boldsymbol{W}] = \boldsymbol{F}\boldsymbol{W}$, the pull-back of which is $\boldsymbol{W} = \chi^*[\boldsymbol{w}] = \boldsymbol{F}^{-1}\boldsymbol{w}$, whereas the push-forward of the material covector $\boldsymbol{Q}$ is the spatial covector $\boldsymbol{q} = \chi_*[\boldsymbol{Q}] = \boldsymbol{F}^{-T}\boldsymbol{Q}$, the pull-back of which is $\boldsymbol{Q} = \chi^*[\boldsymbol{q}] = \boldsymbol{F}^{T}\boldsymbol{q}$. Some push-forward and pull-back operations are particularly important, as they relate the metric with the deformation, and are reported below:

$$\chi_*[\boldsymbol{G}] = \boldsymbol{F}^{-T}\boldsymbol{G}\boldsymbol{F}^{-1} = \boldsymbol{c}^\flat, \tag{1a}$$

$$\chi_*[\boldsymbol{G}^\sharp] = \boldsymbol{F}\boldsymbol{g}^\sharp\boldsymbol{F}^{T} = \boldsymbol{b}^\sharp, \tag{1b}$$

$$\chi^*[\boldsymbol{g}] = \boldsymbol{F}^{T}\boldsymbol{g}\boldsymbol{F} = \boldsymbol{C}^\flat, \tag{1c}$$

$$\chi^*[\boldsymbol{g}^\sharp] = \boldsymbol{F}^{-1}\boldsymbol{g}^\sharp\boldsymbol{F}^{-T} = \boldsymbol{B}^\sharp. \tag{1d}$$

In the undeformed configuration, when the deformation gradient $\boldsymbol{F}$ equals the shifter $\boldsymbol{\Upsilon}$ (in Cartesian coordinates, with collinear material and spatial reference frames, $\bar{F}^i{}_I = \Upsilon^i{}_I = \delta^i_I$), the various deformation tensors seen become

$$\boldsymbol{C} = \boldsymbol{I}, \qquad \boldsymbol{b} = \boldsymbol{i}, \tag{2a}$$

$$\boldsymbol{C}^\flat = \boldsymbol{G}, \qquad \boldsymbol{b}^\sharp = \boldsymbol{g}^\sharp, \tag{2b}$$

$$\boldsymbol{c} = \boldsymbol{i}, \qquad \boldsymbol{B} = \boldsymbol{I}, \tag{2c}$$

$$\boldsymbol{c}^\flat = \boldsymbol{g}, \qquad \boldsymbol{B}^\sharp = \boldsymbol{G}^\sharp. \tag{2d}$$

1.2 *Isotropic and Transversely Isotropic Second-Order Tensors*

Isotropy is the symmetry (invariance) under all possible rotations. Material second-order isotropic tensors are all tensors proportional to the material identity $\boldsymbol{I}$.

Transverse isotropy is the symmetry under rotations about a given direction, called *axial direction*, the plane orthogonal to which (with respect to the given metric) is called *transverse plane*. The subspace of second-order transversely isotropic tensors with respect to a given direction has dimension two. In the case of material tensors, the basis is obtained by decomposing the identity $\boldsymbol{I}$ into $\boldsymbol{I} = \boldsymbol{A} + \boldsymbol{T}$. Tensors $\boldsymbol{A}$ and $\boldsymbol{T}$ are given by

$$\boldsymbol{A} = \boldsymbol{M} \otimes [\boldsymbol{G}\boldsymbol{M}], \tag{3a}$$

$$\boldsymbol{T} = \boldsymbol{I} - \boldsymbol{M} \otimes [\boldsymbol{G}\boldsymbol{M}] = \boldsymbol{I} - \boldsymbol{A}, \tag{3b}$$

where the unit vector $\boldsymbol{M}$ is the axial direction, which gives $\boldsymbol{A}$ and $\boldsymbol{T}$ the geometrical meaning of projection operators on the axial direction and the transverse plane, respectively. Any tensor $\boldsymbol{Y}$ with transverse isotropy with respect to $\boldsymbol{M}$ is written as the linear combination

$$\boldsymbol{Y} = Y^A\boldsymbol{A} + Y^T\boldsymbol{T}. \tag{4}$$

The associated tensors

$$\boldsymbol{A}^\dagger = \boldsymbol{G}\boldsymbol{A}\boldsymbol{G}^\sharp = [\boldsymbol{G}\boldsymbol{M}] \otimes \boldsymbol{M}, \tag{5a}$$

$$\boldsymbol{T}^\dagger = \boldsymbol{G}\boldsymbol{T}\boldsymbol{G}^\sharp = \boldsymbol{I} - [\boldsymbol{G}\boldsymbol{M}] \otimes \boldsymbol{M} = \boldsymbol{I} - \boldsymbol{A}^\dagger, \tag{5b}$$

are the axial and transverse operators for covectors, and their matrix entries are those of $\boldsymbol{A}^T$ and $\boldsymbol{T}^T$, respectively [5].

Walpole [8] defined the axial and transverse operators only in the case of cartesian coordinates, when there is no difference between contravariant and covariant components, and small deformations, when material and spatial picture approximate each other, and in fact he used lowercase letters $\boldsymbol{a}$ and $\boldsymbol{b}$. The same notation has been adopted by Federico and Herzog [2, 3]. Here, the symbol $\boldsymbol{T}$ has been preferred for the transverse operator, for "phonetic" reasons and, above all, in order to avoid confusion with the deformation tensors $\boldsymbol{b}$ and $\boldsymbol{B}$, which may be employed in further developments of the theory, when considering explicit dependence of the permeability on the deformation.

Finally, note that tensor $\boldsymbol{A}^\sharp = \boldsymbol{M} \otimes \boldsymbol{M}$ is commonly called structure tensor or fabric tensor.

1.3 *Spatial and Material Darcy's Law*

The basic form of Darcy's Law is written in spatial form, in terms of the spatial filtration velocity $\boldsymbol{w}$, spatial permeability tensor $\boldsymbol{k}$ and spatial gradient of the pressure, $\operatorname{grad} p = -\boldsymbol{q}$, where the spatial covector field $\boldsymbol{q}$ is the *hydraulic head*:

$$\boldsymbol{w} = -\boldsymbol{k} \operatorname{grad} p = \boldsymbol{k}\, \boldsymbol{q}. \tag{6}$$

A pull-back operation performed on Darcy's law yields its material counterpart:

$$\boldsymbol{W} = -\boldsymbol{K} \operatorname{Grad} p = \boldsymbol{K}\, \boldsymbol{Q}, \tag{7}$$

where $\boldsymbol{W} = \boldsymbol{F}^{-1}\boldsymbol{w}$ is the material filtration velocity, $\boldsymbol{K} = \boldsymbol{F}^{-1}\boldsymbol{k}\boldsymbol{F}^{-T}$ is the material permeability, $\operatorname{Grad} p = \boldsymbol{F}^T \operatorname{grad} p$ is the material gradient of p, $\boldsymbol{Q} = \boldsymbol{F}^T \boldsymbol{q}$ is the material hydraulic head, and use has been made of the identity $\boldsymbol{i} = \boldsymbol{F}^{-T}\boldsymbol{F}^T$.

Note that here the permeability is considered to be a fully contravariant tensor, which is most natural [1]. In order to do this, the venial sin has been committed of considering the gradient to be a covector. Rigorously speaking, use should have been made of the differential $\boldsymbol{d}p$ which is the covector field associated with the vector field $\operatorname{grad} p$ by means of $\boldsymbol{d}p = \boldsymbol{g} \operatorname{grad} p$. If the permeability had been considered as a mixed tensor, with the first index contravariant and the second covariant, then $\operatorname{grad} p$ would have been treated as a vector.

2 METHODS

The microstructural model of permeability under large deformations is based on a homogenisation performed in the material picture, where the arrangement of the fibres is fixed (and known) in the reference configuration. Following the lines of the small-deformation homogenisation procedure described in [2], the material permeability $\boldsymbol{K}$ is obtained as the directional average of the *local* permeability $\boldsymbol{Z}(\boldsymbol{M})$ of an elementary volume containing fluid, matrix, and a fibre oriented in the direction $\boldsymbol{M}$:

$$\boldsymbol{K} = \int_{\mathbb{S}^2} \psi\, \boldsymbol{Z}\, dS. \tag{8}$$

In Equation (8), $\mathbb{S}^2 = \{\boldsymbol{M} \in \mathbb{R}^3 : \|\boldsymbol{M}\| = 1\}$ is the unit sphere (the set of all directions in space) and ψ is a normalised probability density function, such that $\psi(\boldsymbol{M})$ is the probability for a fibre to be in the direction $\boldsymbol{M} \in \mathbb{S}^2$, and $\int_{\mathbb{S}^2} \psi \, dS = 1$. The material permeability tensor $\boldsymbol{K}$ is then pushed forward to the spatial tensor

$$\boldsymbol{k} = \boldsymbol{F}\boldsymbol{K}\boldsymbol{F}^T, \tag{9}$$

which is used in the ordinary spatial Darcy's law (6).

The only difficulty in a Finite Element implementation of the method is programming a user-defined routine that evaluates the spatial permeability tensor $\boldsymbol{k}$ at each simulation increment. The largest part of the problem is in fact the determination of the local permeability $\boldsymbol{Z}(\boldsymbol{M})$.

2.1 *Material Local Permeability*

Based on balance equations for the flow and the pressure gradient [6], the analogy between porous and dielectric media, and Landau and Lifshitz' solution for an impermeable cylinder in a dielectric medium [4], the local permeability for the case of small fibre volumetric fraction has been found for small deformations [2]. For the case of large deformations, and in general coordinates, the equations take a similar form, with the material local permeability $\boldsymbol{Z}_0$ depending on the permeability of the matrix $\boldsymbol{Z}_0$ and the fibre volumetric fraction ϕ, but featuring the tensor $\boldsymbol{Y}^\dagger$, associated with the tensor $\boldsymbol{Y}$ of coefficient of influence via Equations (5), as it has to operate on the covector hydraulic head $\boldsymbol{Q}$:

$$\boldsymbol{Z} = \boldsymbol{Z}_0 \left[\boldsymbol{I} - \phi \boldsymbol{Y}^\dagger\right]. \tag{10}$$

Tensor $\boldsymbol{Y}$ is transversely isotropic in the direction $\boldsymbol{M}$ of the fibre, and given by [4, 2]

$$\boldsymbol{Y} = \boldsymbol{A} + 2\boldsymbol{T}. \tag{11}$$

By means of differential methods for composites with a high volumetric fraction of inclusions [10], it is possible to bring (10) into the differential equation

$$\boldsymbol{Z}'(\Gamma) = -\boldsymbol{Z}(\Gamma)\, \boldsymbol{Y}^\dagger, \tag{12}$$

where Γ is a parameter such that $\phi = 1 - \mathrm{e}^{-\Gamma}$. The solution to Equation (12), with initial condition $\boldsymbol{Z}(0) = \boldsymbol{Z}_0$ (i.e., at zero fibre fraction, the local permeability coincides with that of the matrix), is

$$\boldsymbol{Z}(\Gamma) = \boldsymbol{Z}_0\, \mathrm{e}^{-\Gamma \boldsymbol{Y}^\dagger}. \tag{13}$$

By using the expression (11) of $\boldsymbol{Y}$, and the fact that $\boldsymbol{A}$ and $\boldsymbol{T}$ are idempotent (i.e., $\boldsymbol{A}\boldsymbol{A} = \boldsymbol{A}$ and $\boldsymbol{T}\boldsymbol{T} = \boldsymbol{T}$) and commute (indeed, $\boldsymbol{A}\boldsymbol{T} = \boldsymbol{T}\boldsymbol{A} = \mathbf{O}$), the local permeability becomes

$$\boldsymbol{Z}(\Gamma) = \boldsymbol{Z}_0\, \mathrm{e}^{-\Gamma \boldsymbol{A}^\dagger - 2\Gamma \boldsymbol{T}^\dagger} = \boldsymbol{Z}_0 \left[\mathrm{e}^{-\Gamma} \boldsymbol{A}^\dagger + \mathrm{e}^{-2\Gamma} \boldsymbol{T}^\dagger\right]. \tag{14}$$

Now, recalling that $\Gamma = -\ln(1 - \phi)$, $\boldsymbol{Z}$ can be expressed in terms of the fibre fraction, ϕ:

$$\boldsymbol{Z} = \boldsymbol{Z}_0 \left[(1 - \phi)\boldsymbol{A}^\dagger + (1 - \phi)^2 \boldsymbol{T}^\dagger\right]. \tag{15}$$

By means of the definition of $\boldsymbol{T}$ (Equation (3b)) and some straightforward algebraic manipulation, $\boldsymbol{Z}$ can be put into the alternative forms

$$\boldsymbol{Z} = \boldsymbol{Z}_0 \left[\phi(1 - \phi)\boldsymbol{A}^\dagger + (1 - \phi)^2 \boldsymbol{I}\right], \tag{16}$$

and

$$\boldsymbol{Z} = \phi(1 - \phi)\boldsymbol{Z}_0 \boldsymbol{A}^\dagger + (1 - \phi)^2 \boldsymbol{Z}_0. \tag{17}$$

2.2 *Material Overall Permeability*

The material overall permeability tensor is obtained by substituting the expression (16) of the material local permeability $\boldsymbol{Z}$ into Equation (8):

$$\boldsymbol{K} = \int_{\mathbb{S}^2} \psi\, \boldsymbol{Z}\; dS = \boldsymbol{Z}_0 \left[\phi(1-\phi) \int_{\mathbb{S}^2} \psi\, \boldsymbol{A}^\dagger\; dS + (1-\phi)^2\, \boldsymbol{I} \int_{\mathbb{S}^2} \psi\, dS \right]. \tag{18}$$

Here, tensor $\boldsymbol{A}$ has been considered an explicit function of the direction $\boldsymbol{M}$, i.e., $\boldsymbol{A}(\boldsymbol{M}) = \boldsymbol{M} \otimes [\boldsymbol{G}\boldsymbol{M}]$. By defining the directional average of $\boldsymbol{A}$ as

$$\boldsymbol{H} = \int_{\mathbb{S}^2} \psi\, \boldsymbol{A}\; dS, \tag{19}$$

and using the normalisation condition $\int_{\mathbb{S}^2} \psi\, dS = 1$, Equation (18) becomes

$$\boldsymbol{K} = \boldsymbol{Z}_0 \left[\phi(1-\phi)\, \boldsymbol{H}^\dagger + (1-\phi)^2\, \boldsymbol{I} \right], \tag{20}$$

which admits the alternative form

$$\boldsymbol{K} = \phi(1-\phi)\, \boldsymbol{Z}_0 \boldsymbol{H}^\dagger + (1-\phi)^2\, \boldsymbol{Z}_0. \tag{21}$$

2.3 *Spatial Overall Permeability*

Substitution of Equation (20) into the push-forward (9) yields the spatial overall permeability

$$\begin{aligned} \boldsymbol{k} &= \boldsymbol{F}\, \boldsymbol{Z}_0 \boldsymbol{F}^T\, \boldsymbol{F}^{-T} \left[\phi(1-\phi)\, \boldsymbol{H}^\dagger + (1-\phi)^2\, \boldsymbol{I} \right] \boldsymbol{F}^T, \\ &= \boldsymbol{F}\, \boldsymbol{Z}_0 \boldsymbol{F}^T \left[\phi(1-\phi)\, \boldsymbol{F}^{-T} \boldsymbol{H}^\dagger \boldsymbol{F}^T + (1-\phi)^2\, \boldsymbol{I} \right], \end{aligned} \tag{22}$$

where use has been made of the identity $\boldsymbol{F}^{-1}\boldsymbol{F} = \boldsymbol{I}$. By denoting $\boldsymbol{z}_0$ and $\boldsymbol{h}^\dagger$ the push-forward's of $\boldsymbol{Z}_0$ and $\boldsymbol{H}^\dagger$, respectively, and using Equations (1), the spatial overall permeability takes the form

$$\boldsymbol{k} = \boldsymbol{z}_0 \left[\phi(1-\phi)\, \boldsymbol{h}^\dagger + (1-\phi)^2\, \boldsymbol{i} \right], \tag{23}$$

which can be written in the alternative form

$$\boldsymbol{k} = \phi(1-\phi) \boldsymbol{z}_0 \boldsymbol{h}^\dagger + (1-\phi)^2\, \boldsymbol{z}_0. \tag{24}$$

In the undeformed configuration, when $\boldsymbol{F}$ reduces to the shifter $\boldsymbol{\Upsilon}$, and $\boldsymbol{k}$, $\boldsymbol{z}_0$ and $\boldsymbol{h}^\dagger$ become

$$\mathring{\boldsymbol{k}} = \boldsymbol{\Upsilon} \boldsymbol{K} \boldsymbol{\Upsilon}^T, \tag{25a}$$

$$\mathring{\boldsymbol{z}}_0 = \boldsymbol{\Upsilon} \boldsymbol{K}_0 \boldsymbol{\Upsilon}^T, \tag{25b}$$

$$\mathring{\boldsymbol{h}}^\dagger = \boldsymbol{\Upsilon}^{-T} \boldsymbol{H}^\dagger \boldsymbol{\Upsilon}^T. \tag{25c}$$

The zero-deformation form of Equation (9) is then

$$\mathring{\boldsymbol{k}} = \mathring{\boldsymbol{z}}_0 \left[\phi(1-\phi)\, \mathring{\boldsymbol{h}}^\dagger + (1-\phi)^2\, \boldsymbol{i} \right]. \tag{26}$$

In Cartesian coordinates, the difference between $\mathring{\boldsymbol{h}}^\dagger$ and $\mathring{\boldsymbol{h}}$ drops, and Equation (26) reads

$$\mathring{\boldsymbol{k}} = \mathring{\boldsymbol{z}}_0 \left[\phi(1-\phi)\, \mathring{\boldsymbol{h}} + (1-\phi)^2\, \boldsymbol{i} \right], \tag{27}$$

which is equivalent to Equation (4.6) in the work by Federico and Herzog [2], obtained for the case of isotropic (material) matrix permeability $\boldsymbol{Z}_0$ and small deformations (with suitable changes in the symbols: $\mathring{\boldsymbol{k}} \to \boldsymbol{K}$, $\mathring{\boldsymbol{z}}_0 \to \boldsymbol{k}_0$, $\mathring{\boldsymbol{h}} \to \boldsymbol{Q}$, $\boldsymbol{i} \to \boldsymbol{I}$).

3 DISCUSSION

This expression generalises the result obtained in [2] for the case of matrix with isotropic permeability. In the general case, unless $\boldsymbol{Z}_0$ is coaxial with $\boldsymbol{G}^\sharp[(1-\phi)\boldsymbol{A}^\dagger + (1-\phi)^2\boldsymbol{T}^\dagger]$ (Equation (15)), the local permeability $\boldsymbol{Z}$ is *non-symmetric*, which is reflected in the non-symmetry of the overall permeability tensor $\boldsymbol{K}$ (Equation (8)). This non-symmetry, arising from a homogenisation procedure, is similar to that found in the overall elasticity tensor of a composite with aligned spheroidal inclusions phases with different aspect ratio [7]. In that case, a "brute force solution" was proposed, consisting in simply neglecting the non-symmetric part of the elasticity tensor [9]. Here, the equivalent would be to symmetrise $\boldsymbol{K}$ before calculating its spatial counterpart $\boldsymbol{k}$ (Equation (9)). However, the physical soundness of a non-symmetric permeability tensor requires further investigation. In contrast, the hypothesis of large deformations implies solely the difficulty of programming a user-routine in the Finite Element implementation, in order to obtain the spatial permeability as the push-forward of the material permeability.

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