A FINITE ELEMENT IMPLEMENTATION OF KNOWLES STORED-ENERGY FUNCTION: THEORY, CODING AND APPLICATIONS

This paper contains the full way of implementing a user-defined hyperelastic constitutive model into the finite element method (FEM) through defining an appropriate elasticity tensor. The Knowles stored-energy potential has been chosen to illustrate the implementation, as this particular potential function proved to be very effective in modeling nonlinear elasticity within moderate deformations. Thus, the Knowles stored-energy potential allows for appropriate modeling of thermoplastics, resins, polymeric composites and living tissues, such as bone for example. The decoupling of volumetric and isochoric behavior within a hyperelastic constitutive equation has been extensively discussed. An analytical elasticity tensor, corresponding to the Knowles stored-energy potential, has been derived. To the best of author’s knowledge, this tensor has not been presented in the literature yet. The way of deriving analytical elasticity tensors for hyperelastic materials has been discussed in detail. The analytical elasticity tensor may be further used to develop visco-hyperelastic, nonlinear viscoelastic or viscoplastic constitutive models. A FORTRAN 77 code has been written in order to implement the Knowles hyperelastic model into a FEM system. The performance of the developed code is examined using an exemplary problem.

NOMENCLATURE

\( \mathbf{B} \) left Cauchy-Green (C-G) deformation tensor,
\( \mathbf{\overline{B}} \) isochoric left C-G deformation tensor,
\( \mathbf{B}_l, \mathbf{B}_t \) reference and current configurations,
\( \mathbf{B}^{\omega} \) current configuration after purely distortional deformation,
\( \mathbf{C} \) right Cauchy-Green (C-G) deformation tensor,
\( \mathbf{\overline{C}} \) isochoric right C-G deformation tensor,
\( \mathbf{C} \) elasticity tensor,
\( \mathbf{C}^{\omega} \) elasticity tensor related to convected stress rate.

* Warsaw University of Technology, Institute of Mechanics and Printing, ul. Narbutta 85, 02-524 Warszawa, Poland; E-mail: csuchocki@o2.pl
1. Introduction

Numerous materials such as thermoplastics, resins or polymeric composites exhibit nonlinear elastic behavior for strains ranging up to 5%. In order to take this phenomenon into account in the Finite Element Analysis (FEA), a proper hyperelastic constitutive model has to be employed.

As it has been observed by several researchers [3], [21], the popular models of hyperelasticity like Neo-Hooke or Mooney-Rivlin for instance, which are very effective in modeling large strain nonlinear elasticity, are not able to capture the nonlinear elastic behavior in the range up to 5%. This problem is usually skipped by making use of the linear elastic model (Saint-Venant-Kirchhoff stored-energy potential) or/and assuming that the entire nonlinearity is due to plasticity. This assumption is in contradiction to the experimental observations. In the case of thermoplastic polymers for example, it can be noticed that after a loading-unloading experiment a certain strain
remains in the specimen in face of a zero stress. It should be noticed, however, that the remaining strain is not plastic but viscoelastic, and it decreases as the specimen rests, to finally vanish after a properly long time period. This kind of behavior is typical for viscoelastic materials, and it is usually stated that this group of materials does not possess a well-defined stress free state. In other words, the stress free state of the specimen may occur at different states of deformation. Since the deformations are elastic, they should be modeled as such, and assuming that they are plastic is a mistake.

Fig. 1. Simple tension test data and theoretical predictions

It has been already mentioned that the popular models of hyperelasticity fail to capture the experimental stress-strain curve of the materials which exhibit nonlinear elasticity for moderate strains. The theoretical predictions of Saint Venant-Kirchhoff (S V-K), Neo-Hooke (N-H) and Knowles (K) models are compared in the Figure 1 to the experimental results of a simple tension test performed on a specimen of high density polyethylene [7]. A proper set of material constants can allow for good description of small strain behavior, as it can be seen for the Saint Venant-Kirchhoff model. Further predictions carry a significant error which can range over 50%. Improving the model predictions for higher strains results in increasing the error in the range of small strains, as it has been shown for Neo-Hooke model. Thus, a stored-energy potential that would effectively describe the stress-strain relation is needed. For that purpose several researchers have proposed various, alternative stored-energy potentials. Bouchart proposed using Ciarlet-Geymonat stored-energy function in order to model the elastic response of polypropylene [3]. This model uses four material constants and all three invariants of the right Cauchy-Green (C-G) deformation tensor. It appears that Knowles stored-energy potential [11], used by Soares and Rajagopal to model poly-lactide [22], is a better solution. The model by Knowles uses four material
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constants but only one invariant (first) of the right C-G deformation tensor which simplifies the process of material parameter identification. As it can be seen in Figure 1, the Knowles model allows for effective modeling of elastic response of thermoplastics, resins, polymeric composites, metals and living tissues such as bone for example.

The model by Knowles is not offered by any of the popular FEA systems and, in order to use it, one has to implement it as a user-defined material. In this study, the full way of implementing the Knowles material model into FEA system Abaqus has been presented. The focus on Abaqus system does not cause a loss in generality as the general framework of implementing a user-defined material is similar in all FEA systems.

A user-defined hyperelastic constitutive laws can be implemented into Abaqus in several ways. Abaqus offers three alternative user subroutines which can be used for implementing a hyperelastic constitutive equation. Those are: UHYPER (for isotropic incompressible hyperelastic materials), UANISOHYPER (for anisotropic hyperelastic materials) and UMAT (general purpose subroutine which can be used for implementing arbitrary material behavior). Abaqus allows for using both UHYPER and UANISOHYPER to develop a more sophisticated constitutive equations. Both subroutines can be used to model nonlinear viscoelasticity within a theory which is similar to the Pipkin & Rogers theory of viscoelasticity [5]. Alternatively, Mullins effect can be modeled together with the elastic response defined by a user subroutine (viscoelasticity and Mullins effect must be used separately; Abaqus does not allow for combining those behaviors). Thus, a user implementing his constitutive equation through subroutines UHYPER or UANISOHYPER is limited to using built-in options of Abaqus.

In order to develop a constitutive equation based on the theories not supported by Abaqus, subroutine UMAT should be used. Using subroutine UMAT requires defining material stiffness tensor also referred to as tangent modulus tensor, material Jacobian or elasticity tensor in the case of elastic materials. The derivation of an analytical elasticity tensor is not an easy task, which is the reason why the approximate elasticity tensors are often used, although they worsen the rate of convergence and accuracy of analysis' results. Stein and Sagar [23] have found for the Neo-Hooke hyperelastic model that only an analytically derived elasticity tensor assures a quadratic rate of convergence\(^1\). For the approximate elasticity tensors, not only the convergence rates are not quadratic but even convergence at all is not assured.

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\(^1\) Quadratic convergence means that the square of the error at one iteration is proportional to the error at the next iteration.
for all elements and considered problems. Thus, it is always profitable to use an analytical elasticity tensor whenever it is possible.

This paper presents the entire way of derivation of an analytical elasticity tensor corresponding to the Knowles stored-energy potential. To the best of author’s knowledge, this tensor has not been reported in the literature yet. It should be noted that the discussed framework is valid for both isotropic and anisotropic hyperelastic materials.

2. Kinematics of finite deformations

Let us consider a continuum body whose reference configuration is denoted as $B_r$. As a consequence of the deformation, the body takes a new (current) configuration denoted as $B_t$ (Fig. 2).

![Fig. 2. Deformation gradient $F$](image)

The position vectors of a considered particle are denoted as $X$ and $x$ in the reference and current configurations, respectively. It is assumed that a one-to-one mapping function of the form $x = \chi(X, t)$ exists.

The deformation gradient $F$ is a second-order tensor which is defined by the following equation:

$$F = \text{Grad} \chi(X, t)$$

where “Grad” denotes a gradient operation with respect to the components of vector $X$. The Cartesian components of $F$ are $F_{ij} = \partial x_i / \partial X_j$ (i, j = 1, 2, 3).

During the motion, a spatial velocity field may be expressed as $v(x, t) = \partial x / \partial t$ and a velocity gradient tensor can be defined as $L = FF^{-1}$. As any other second-order tensor, $L$ can be decomposed into a sum of a symmetric and an antisymmetric tensors, namely $L = D + W$, where $D = \frac{1}{2}(L + L^T)$ is the strain rate tensor and $W = \frac{1}{2}(L - L^T)$ is the spin tensor. The symmetric
Fig. 3. Alternative paths of deformation

and positive-definite right and left Cauchy-Green (C-G) deformation tensors are defined as $C = F^T F$ and $B = FF^T$, respectively.

For the use of finite element method it is worthy to decouple the dilatational (volumetric) and distortional (isochoric) deformations. This can be achieved by a multiplicative decomposition of the deformation gradient [9]:

$$ F = F_{vol} \bar{F} $$

where $F_{vol}$ denotes a deformation gradient corresponding to purely volumetric deformation ($F_{vol} = J^{1/3} I$) and $\bar{F}$ denotes a deformation gradient corresponding to purely isochoric deformation ($\bar{F} = J^{-1/3} F$). $J = \det F$ is the Jacobian determinant also known as the volume ratio. Figure 3 provides a graphic interpretation of the considered multiplicative decomposition. Other deformation tensors can be decomposed in a similar way. The right and left Cauchy-Green (C-G) deformation tensors are decomposed as [9]:

$$ C = F^T F = J^{2/3} \overline{C}, \quad B = FF^T = J^{2/3} \overline{B} $$

where $\overline{C} = \bar{F}^T \bar{F}$ and $\overline{B} = \bar{F}F^T$ are the right and left volume-preserving C-G deformation tensors, respectively.

3. Decoupled constitutive equation of hyperelastic material

A hyperelastic or Green elastic material is defined as an elastic material which possesses a stored elastic energy function, denoted as $W_e$ [9], [15], [16].
From the principles of conservation of energy and conservation of angular momentum the following expression for the time derivative of the stored-energy potential can be obtained \[24\]:

$$
\dot{W}_e = \mathbf{S} \cdot \dot{\mathbf{E}} = \frac{1}{2} \mathbf{S} \cdot \dot{\mathbf{C}}
$$

(4)

where \( \mathbf{S} \) is the second Piola-Kirchhoff (P-K) stress tensor, \( \mathbf{E} \) is the Green finite strain tensor and \( \mathbf{C} \) is the right Cauchy-Green (C-G) deformation tensor. After assuming that \( W_e = W_e(C) \) and applying the chain rule to (4), it is found that:

$$
\left( \mathbf{S} - 2 \frac{\partial W_e}{\partial \mathbf{C}} \right) \cdot \frac{1}{2} \dot{\mathbf{C}} = 0
$$

(5)

which holds for arbitrary \( \dot{\mathbf{C}} \). Thus it can be deduced that:

$$
\mathbf{S} = 2 \frac{\partial W_e}{\partial \mathbf{C}}
$$

(6)

which is the general form of the constitutive equation determining the relation between stress and deformation tensors for a hyperelastic material.

For the isotropic hyperelastic materials, \( W_e \) may be regarded as a function of the three principal algebraic invariants \( I_1, I_2, I_3 \) of \( \mathbf{C} \), namely:

$$
W_e(C) = W_e(I_1, I_2, I_3)
$$

(7)

in order to fulfill the requirements of objectivity and isotropy.

The invariants of the right C-G deformation tensor are given by the following formulas:

$$
I_1 = \text{tr} \, \mathbf{C}, \quad I_2 = \frac{1}{2} \left( (\text{tr} \, \mathbf{C})^2 - \text{tr} \, \mathbf{C}^2 \right), \quad I_3 = J^2 = \det \mathbf{C}
$$

(8)

where \( \text{tr} (\bullet) \) is the trace operator and \( J \) is the Jacobian determinant.

In terms of FEM, it is profitable if the volumetric and isochoric responses are decoupled within the constitutive equation. The decoupling significantly simplifies the derivation and the final form of the fourth-order elasticity tensor. It is facilitated by assuming a stored-energy function of the form \[9\], \[25\]:

$$
W_e(C) = U(J) + \overline{W}(\overline{C})
$$

(9)

where \( U \) and \( \overline{W} \) are volumetric and isochoric stored-energy potentials, respectively. The enforcement of incompressibility constraint is much easier for an uncoupled stored-energy, as it is achieved simply by assuming a properly high value of the bulk modulus.
In order to find a general form of a constitutive equation corresponding to a stored-energy potential given by (9), the following results are needed:

$$\frac{\partial J}{\partial C} = \frac{1}{2} J C^{-1}, \quad \frac{\partial \overline{C}}{\partial C} = J^{-2/3}\left(I - \frac{1}{3} C \otimes C^{-1}\right).$$  \hfill (10)

By substituting stored-energy potential (9) into (6), making use of the chain rule and the results (10), it is in turn found that:

$$S = 2 \frac{\partial U}{\partial J} \frac{\partial J}{\partial C} + 2 \frac{\partial \overline{W}}{\partial C} \cdot \frac{\partial \overline{C}}{\partial C}$$

$$= J \frac{\partial U}{\partial J} C^{-1} + 2 J^{-2/3} \frac{\partial \overline{W}}{\partial C} \left(I - \frac{1}{3} \overline{C} \otimes \overline{C}^{-1}\right)$$

$$= J \frac{\partial U}{\partial J} C^{-1} + 2 J^{-2/3} \left[ \frac{\partial \overline{W}}{\partial C} - \frac{1}{3} \left( \frac{\partial \overline{W}}{\partial C} \cdot \overline{C} \right) \overline{C}^{-1} \right]$$

After introducing the following operator [25]:

$$\text{DEV} [\bullet] = [\bullet] - \frac{1}{3} \left( [\bullet] \cdot \overline{C} \right) \overline{C}^{-1}$$  \hfill (11)

which extracts the deviatoric part from a second order tensor in the reference configuration, the above lengthty result can be significantly shortened, that is:

$$S = J \frac{\partial U}{\partial J} C^{-1} + 2 J^{-2/3} \text{DEV} \left[ \frac{\partial \overline{W}}{\partial C} \right].$$  \hfill (12)

It should be emphasized that the equation (12) is valid for both isotropic and anisotropic materials.

In the special case of the isotropic hyperelastic materials, the stored-energy potential takes the form:

$$W_e(C) = U(J) + \overline{W}(\overline{I}_1, \overline{I}_2)$$  \hfill (13)

where $\overline{I}_1 = J^{-2/3} I_1$ and $\overline{I}_2 = J^{-4/3} I_2$. Depending on the values of the material parameters associated with the volumetric potential $U(J)$, equation (12) can describe compressible, slightly compressible or almost-incompressible material.
4. Uncoupled elasticity tensor and objective rate of stress tensor

The nonlinear constitutive equation defined by (6) can be transformed into the following incremental form [2], [9], [14]:

\[ \Delta S = \mathbf{C} \cdot \frac{1}{2} \Delta \mathbf{C} \]  

(14)

which is a linear relation between the increments of \( S \) and \( C \), and so it is commonly referred to as linearized constitutive equation. \( \mathbf{C} \) denotes a fourth-order elasticity tensor, defined as:

\[ \mathbf{C} = 2 \frac{\partial S}{\partial \mathbf{C}} = 4 \frac{\partial^2 W_e}{\partial \mathbf{C} \partial \mathbf{C}}. \]  

(15)

Substituting the equation (12) into (15) gives [25]:

\[ \mathbf{C} = 2 \frac{\partial S}{\partial \mathbf{C}} = 2 \frac{\partial}{\partial \mathbf{C}} \left( 2 \frac{\partial W_e}{\partial \mathbf{C}} \right) = 2 \frac{\partial}{\partial \mathbf{C}} \left\{ J \frac{\partial U}{\partial J} \mathbf{C}^{-1} + 2J^{-2/3} \left[ \frac{\partial W}{\partial \mathbf{C}} - \frac{1}{3} \left( \frac{\partial W}{\partial \mathbf{C}} \cdot \mathbf{C}^{-1} \right) \right] \right\}. \]  

(16)

Having in mind the results (10) and additionally \( \frac{\partial \mathbf{C}^{-1}}{\partial \mathbf{C}} = -\mathbf{I}_{\mathbf{C}^{-1}} \), where \( (\mathbf{I}_{\mathbf{C}^{-1}})_{ijkl} = -\frac{1}{2} \left( \mathbf{C}^{-1}_{ik} \mathbf{C}^{-1}_{jl} + \mathbf{C}^{-1}_{il} \mathbf{C}^{-1}_{jk} \right) \), a systematic use of the chain rule leads to an expression³:

\[ \mathbf{C} = J \frac{\partial U}{\partial J} \left( \mathbf{C}^{-1} \otimes \mathbf{C}^{-1} - 2\mathbf{I}_{\mathbf{C}^{-1}} \right) + J^2 \frac{\partial^2 U}{\partial J^2} \mathbf{C}^{-1} \otimes \mathbf{C}^{-1} \]

\[ - \frac{4}{3}J^{-4/3} \left( \frac{\partial W}{\partial \mathbf{C}} \otimes \mathbf{C}^{-1} + \mathbf{C}^{-1} \otimes \frac{\partial W}{\partial \mathbf{C}} \right) \]

\[ + \frac{4}{3}J^{-4/3} \left( \frac{\partial W}{\partial \mathbf{C}} \cdot \mathbf{C} \right) \left( J^{4/3} \mathbf{I}_{\mathbf{C}^{-1}} + \frac{1}{3} \mathbf{C}^{-1} \otimes \mathbf{C}^{-1} \right) + J^{-4/3} \mathbf{C}_W \]

(17)

² Starting off from this section some differentials met in the formulas have been replaced with finite increments as they are implemented as such into FEM.
³ see Appendix B. for the derivation.
where $\bar{C}_W$ is the part of $C$ which arises directly from the second derivatives of $\bar{W}$ with respect to $\bar{C}$ [25]. It is defined as:

$$
\bar{C}_W = 4 \frac{\partial^2 \bar{W}}{\partial \bar{C} \partial \bar{C}} - \frac{4}{3} \left[ \left( \frac{\partial^2 \bar{W}}{\partial \bar{C} \partial \bar{C}} \cdot \bar{C} \right) \otimes \bar{C}^{-1} + \bar{C}^{-1} \otimes \left( \bar{C} \cdot \frac{\partial^2 \bar{W}}{\partial \bar{C} \partial \bar{C}} \right) \right]
+ \frac{4}{9} \left( \bar{C} \cdot \frac{\partial^2 \bar{W}}{\partial \bar{C} \partial \bar{C}} \cdot \bar{C} \right) \bar{C}^{-1} \otimes \bar{C}^{-1}.
$$

(18)

The incremental constitutive equation (14) which is formulated in the reference configuration can be transformed into the current configuration\(^4\).

It takes the following form [2], [23]:

$$
\mathcal{L}_\tau \tau = \Delta \tau - \left( \Delta \bar{F}^{-1} \right) \tau - \tau \left( \Delta \bar{F}^{-1} \right)^T = \mathcal{C}^{\tau c} \cdot \Delta D
$$

(19)

where $\mathcal{L}_\tau \tau = \Delta \tau - \left( \Delta \bar{F}^{-1} \right) \tau - \tau \left( \Delta \bar{F}^{-1} \right)^T$ is the incremental form of the convected objective rate (also called the Oldroyd or Lie rate) of the Kirchhoff stress $\tau$ and $\mathcal{C}^{\tau c}$ is a transformed elasticity tensor whose components are defined as $\mathcal{C}^{\tau c}_{ijkl} = F_{ip}F_{jq}F_{kr}F_{ls}C_{pqrs}$.

The convected objective rate used to be employed in older versions of Abaqus system. Nowadays Abaqus makes use of the incremental form of the Zaremba-Jaumann\(^5\) objective rate defined as $\tau^Z = \Delta \tau - \Delta \bar{W} \tau - \tau \Delta \bar{W}^T$, and, consequently, a proper incremental constitutive equation takes the form:

$$
\tau^Z = \Delta \tau - \Delta \bar{W} \tau - \tau \Delta \bar{W}^T = \mathcal{C}^{\tau Z-J} \cdot \Delta D
$$

(20)

where

$$
\Delta \bar{W} = \frac{1}{2} \left( \Delta \bar{F}^{-1} - \left( \Delta \bar{F}^{-1} \right)^T \right),
$$

(21)

$$
\Delta D = \frac{1}{2} \left( \Delta \bar{F}^{-1} + \left( \Delta \bar{F}^{-1} \right)^T \right)
$$

(22)

and the elasticity tensor $\mathcal{C}^{\tau Z-J}$ corresponding to the Zaremba-Jaumann objective rate of the Kirchhoff stress is defined as:

\(^4\) see Appendix A. for the derivation.

\(^5\) This kind of objective rate is usually called the Jaumann rate, although it was Polish professor S. Zaremba who introduced it first [19]. The popularity of the name “Jaumann rate” is probably due to unawareness of Zaremba’s works, however, some authors use the name “Jaumann-Zaremba rate” [9]. Through this text the name “Zaremba-Jaumann objective rate” is used.
\[ C^{vZ-J} = C^{rc} + \frac{1}{2} \left( \delta_{ik} \tau_{jl} + \tau_{ik} \delta_{jl} + \delta_{il} \tau_{jk} + \tau_{il} \delta_{jk} \right) e_i \otimes e_j \otimes e_k \otimes e_l \]  
\tag{23}

where \( e_k \) \((k = 1, 2, 3)\) denotes a unit vector of a Cartesian basis.

It should be noted that the elasticity tensor which should be implemented into the subroutine UMAT is slightly different from (23) and takes the form:

\[ C^{MZ-J} = \frac{1}{J} C^{vZ-J}. \]  
\tag{24}

The framework presented above can be used to derive the analytical elasticity tensors of both isotropic and anisotropic hyperelastic materials.

5. Abaqus implementation

5.1. General

In the following text the analytical elasticity tensor following from the Knowles hyperelastic model is presented. The derived analytical elasticity tensor has been implemented into the Abaqus system via subroutine UMAT.

5.2. Application of Knowles stored-energy function

The decoupled form of the Knowles stored-energy function is given as follows [11]:

\[ W_e = \frac{\mu}{2b} \left\{ \left[ 1 + \frac{b}{n} (\bar{I}_1 - 3) \right]^n - 1 \right\} + \frac{1}{D_1} (J - 1)^2 \]  
\tag{25}

where \( \mu \) is a shear modulus, \( n \) is a “hardening” parameter (the material hardens or softens according as \( n > 1 \) or \( n < 1 \)), \( b \) is an additional parameter which improves curve-fitting and \( D_1 \) is the inverse of a bulk modulus [11], [12], [13]. The simplest possible form of the volumetric stored-energy function, namely \( U = \frac{1}{D_1} (J - 1)^2 \), has been assumed. It is easy to notice that \( n = 1 \) and \( b = 1 \) corresponds to the special case of Neo-Hookean solid.

By making use of (12) and the transformation rule \( \tau = F \sigma F^T \), an expression for the Kirchhoff stress is found, that is:

\[ \tau = \frac{2}{D_1} J (J - 1) \mathbf{1} + \mu \left[ 1 + \frac{b}{n} (\bar{I}_1 - 3) \right]^{n-1} \left( \mathbf{B} - \frac{1}{3} \bar{I}_1 \mathbf{1} \right). \]  
\tag{26}
Subsequent use of (17), the transformation rule $C^{σc}_{ijkl} = F_{ip}F_{jq}F_{kl}F_{rs}C_{pqr},$ (23) and (24) leads to the following elasticity tensor expressed by means of Eulerian variables:

$$C^{MZ−J}_{ijkl} = \frac{μ}{J} \left[ 1 + \frac{b}{n} (I_1 - 3) \right]^{n-1} \left[ \frac{1}{2} \left( \delta_{ij} \bar{B}_{jk} + \delta_{jk} \bar{B}_{il} + \delta_{jl} \bar{B}_{ik} + \delta_{ik} \bar{B}_{lj} \right) \right]$$

$$+ \delta_{ij} \bar{B}_{jk} + \delta_{jl} \bar{B}_{ik} + \delta_{ij} \bar{B}_{kl}$$

$$+ \frac{2}{3} \frac{b(n-1)}{n} \left[ 1 + \frac{b}{n} (I_1 - 3) \right]^{n-2} \left[ \bar{B}_{ij} \bar{B}_{kl} - \frac{1}{3} I_3 \bar{B}_{ij} \delta_{kl} \right]$$

$$+ \bar{B}_{ij} \delta_{kl} \right] + \frac{2}{D_1} (2J-1) \delta_{ij} \delta_{kl}.$$  \hspace{1cm} (27)

To the best of author’s knowledge, this elasticity tensor has not been presented in the literature yet. It is further utilized to develop a FORTRAN 77 code allowing one to use the Knowles hyperelastic material model in the FEA system Abaqus and to extend it employing an arbitrary theory.

5.3. Dimensions

In the discussed case of the Knowles hyperelastic material, the elasticity tensor is symmetric and thus it can be degraded to a $6 \times 6$ matrix. Consequently, both the Kirchhoff stress tensor $\tau$ and the isochoric left C-G deformation tensor $\bar{B}$ can be degraded to $6 \times 1$ column vectors. For the tensor $\bar{B}$ the column vector takes the form $\left[ \bar{B}_{ij} \right] = \left[ \bar{B}_{11} \bar{B}_{22} \bar{B}_{33} \bar{B}_{12} \bar{B}_{13} \bar{B}_{23} \right]^T$. Thus the components of the vector denoted by „1”, „2”, ... , „6” correspond to „11”, „22”, ... , „23” components of the tensor, respectively. This rule is employed for the Kirchhoff stress tensor as well. The components of the $6 \times 6$ elasticity matrix $[C_{ij}]$ are equal to the proper components of the elasticity tensor $C^{MZ−J}$. The indices „i” and „j” used in $[C_{ij}]$ refer to the proper tensor indices, determined by the rule described above.

5.4. Variables

In the following table the meaning of the variables used in the FORTRAN code has been explained. The lengthy definitions of the secondary variables have been skipped.

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6 see Appendix C. for the derivation.
Number of direct stress components  
Number of shear stress components  
Constants $\mu$, $b$, $n$ and $D_1$  
Deformation Gradient Tensor $F$  
Jacobian Determinant  
Isochoric Deformation Gradient Tensor $\overline{F}$  
Isochoric Left C-G Deformation Tensor $\overline{B}$  
Trace of $\overline{B}$ divided by 3  
Cauchy Stress Tensor $\sigma$  
Elasticity Matrix  
Secondary Variables

$\text{NDI}$  
$\text{NSHR}$  
$\text{MU, B, N, D1}$  
$\text{DFGRD1(I,J)}$  
$\text{DET}$  
$\text{DISTGR(I,J)}$  
$\text{BBAR(I)}$  
$\text{TRBBAR}$  
$\text{STRESS(I)}$  
$\text{DDSDDE(I,J)}$  
$\text{EK, PR, SCALE, TERM1, TERM2}$

5.5. User Subroutine

Algorithm for the implementation in ABAQUS

Input data: $F$, NDI, NSHR
1. Calculate Jacobian determinant $J$
   
   $$J = \det F$$

2. Calculate isochoric deformation gradient $\overline{F}$
   
   $$\overline{F} = J^{-1/3}F$$

3. Calculate isochoric left C-G deformation tensor $\overline{B}$
   
   $$\overline{B} = FF^T$$

4. Calculate Cauchy stress matrix $\text{STRESS(I)} = \sigma$
   
   $$\sigma = \frac{2}{D_1} (J - 1) 1 + \frac{\mu}{J} \left[ 1 + \frac{b}{n} (\overline{I}_1 - 3) \right]^{n-1} \left( \overline{B} - \frac{1}{3} \overline{I}_1 1 \right)$$

5. Calculate Elasticity Matrix $C_{ij} (DDSDDE(I,J))$ according to (5.3).
5.6. Coding in FORTRAN 77

SUBROUTINE UMAT(STRESS,STATEV,DDSDDE,SSE,SPD,SCD,
1 RPL,DDSDDT,DRPLDE,DRPLDT,STRAN,DSTRAN,
2 TIME,DTIME,TEMP,DTEMP,PREDEF,DPRED,MATERL,NDL,NSHR,NTENS,
3 NSTATV,PROPS,NPROPS,COORDS,DROT,PNEWDT,CELENT,
4 DFGRD0,DFGRD1,NOEL,NPT,KSLAY,KSPRT,KSTEP,KINC)
C
INCLUDE 'ABA_PARAM.INC'
C
CHARACTER*8 MATERL
DIMENSION STRESS(NTENS),STATEV(NSTATV),
1 DDSDDE(NTENS,NTENS),DDSDDT(NTENS),DRPLDE(NTENS),
2 STRAN(NTENS),DSTRAN(NTENS),DFGRD0(3,3),DFGRD1(3,3),
3 TIME(2),PREDEF(1),DPRED(1),PROPS(NPROPS),COORDS(3),DROT(3,3)
C
C LOCAL ARRAYS
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C BBAR - DEVIATORIC RIGHT CAUCHY-GREEN TENSOR
C DISTGR - DEVIATORIC DEFORMATION GRADIENT (DISTORTION TENSOR)
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

DIMENSION BBAR(6),DISTGR(3,3)
C
PARAMETER(ZERO=0.D0, ONE=1.D0, TWO=2.D0, THREE=3.D0, FOUR=4.D0)
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C UMAT FOR COMPRESSIBLE KNOWLES HYPERELASTICITY
C
C WARSAW UNIVERSITY OF TECHNOLOGY
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C CYPRIAN SUCHOCKI, MAY 2011
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C FOR LOW D1 HYBRID ELEMENTS SHOULD BE USED
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C PROPS(1) - MU
C PROPS(2) - B
C PROPS(3) - N
C PROPS(4) - D1
C
C REAL MU, B, N, D1, TERM1, TERM2
C
C ELASTIC PROPERTIES
C
MU=264.069
B=54.19
N=0.2554
D1 =0.000000033
C
C JACOBIAN AND DISTORTION TENSOR
C
DET=DFGRD1(1, 1 )*DFGRD1(2, 2 )*DFGRD1(3, 3)
1 -DFGRD1(1, 2 )*DFGRD1(2, 1 )*DFGRD1(3, 3)
IF(NSHR.EQ.3) THEN
DET=DET+DFGRD1(1, 2 )*DFGRD1(2, 3 )*DFGRD1(3, 1)
1 +DFGRD1(1, 3 )*DFGRD1(3, 2 )*DFGRD1(2, 1)
2 -DFGRD1(1, 3 )*DFGRD1(3, 1 )*DFGRD1(2, 2)
3 -DFGRD1(2, 3 )*DFGRD1(3, 2 )*DFGRD1(1, 1)
A FINITE ELEMENT IMPLEMENTATION...

END IF
SCALE=DET**(-ONE/THREE)
DO K1=1, 3
  DO K2=1, 3
    DISTGR(K2, K1)=SCALE*DFGRD1(K2, K1)
  END DO
END DO

C CALCULATE LEFT CAUCHY-GREEN TENSOR
C
BBAR(1)=DISTGR(1, 1)**2+DISTGR(1, 2)**2+DISTGR(1, 3)**2
BBAR(2)=DISTGR(2, 1)**2+DISTGR(2, 2)**2+DISTGR(2, 3)**2
BBAR(3)=DISTGR(3, 3)**2+DISTGR(3, 1)**2+DISTGR(3, 2)**2
BBAR(4)=DISTGR(1, 1)*DISTGR(2, 1)+DISTGR(1, 2)*DISTGR(2, 2)
  +DISTGR(1, 3)*DISTGR(2, 3)
IF(NSHR.EQ.3) THEN
  BBAR(5)=DISTGR(1, 1)*DISTGR(3, 1)+DISTGR(1, 2)*DISTGR(3, 2)
  +DISTGR(1, 3)*DISTGR(3, 3)
  BBAR(6)=DISTGR(2, 1)*DISTGR(3, 1)+DISTGR(2, 2)*DISTGR(3, 2)
  +DISTGR(2, 3)*DISTGR(3, 3)
END IF

C CALCULATE THE STRESS
C
TRBBAR=(BBAR(1)+BBAR(2)+BBAR(3))/THREE
TERM1=MU/DET*(ONE+B/N*(THREE*TRBBAR-THREE))**(N-ONE)
TERM2=TWO*MU/DET*B*(N-ONE)/N*(ONE+B/N*(THREE*TRBBAR-THREE))**(N-ONE)
EK=TWO/D1*(TWO*DET-ONE)
PR=TWO/D1*(DET-ONE)
DO K1=1,NDI
  STRESS(K1)=TERM1*(BBAR(K1)-TRBBAR)+PR
END DO
DO K1=NDI+1,NDI+NSHR
  STRESS(K1)=TERM1*BBAR(K1)
END DO

C CALCULATE THE STIFFNESS
C
EG23=EG*TWO/THREE
DDSDDE(1, 1)=TWO/THREE*TERM1*(BBAR(1)+TRBBAR)+TERM2*(BBAR(1)**2-TWO*BBAR*TRBBAR+TRBBAR**2)+EK
DDSDDE(2, 2)=TWO/THREE*TERM1*(BBAR(2)+TRBBAR)+TERM2*(BBAR(2)**2-TWO*BBAR*TRBBAR+TRBBAR**2)+EK
DDSDDE(3, 3)=TWO/THREE*TERM1*(BBAR(3)+TRBBAR)+TERM2*(BBAR(3)**2-TWO*BBAR*TRBBAR+TRBBAR**2)+EK
DDSDDE(1, 2)=TWO/THREE*TERM1*(BBAR(1)+TRBBAR)+TERM2*(BBAR(1)*BBAR(2)-TRBBAR*BBAR(2)+TRBBAR**2)+EK
DDSDDE(1, 3)=TWO/THREE*TERM1*(BBAR(1)+TRBBAR)+TERM2*(BBAR(1)*BBAR(3)-TRBBAR*BBAR(3)+TRBBAR**2)+EK
DDSDDE(2, 3)=TWO/THREE*TERM1*(BBAR(2)+TRBBAR)+TERM2*(BBAR(2)*BBAR(3)-TRBBAR**2)+EK
DDSDDE(1, 4)=TWO/THREE*TERM1*(BBAR(1)+TRBBAR)+TERM2*(BBAR(1)*BBAR(4)-TRBBAR*BBAR(4)+TRBBAR**2)+EK
DDSDDE(2, 4)=TWO/THREE*TERM1*(BBAR(2)+TRBBAR)+TERM2*(BBAR(2)*BBAR(4)-TRBBAR**2)+EK

6. Performance

In order to verify the performance of the code presented above, a simulation of a uniaxial tension experiment has been conducted in FEA system Abaqus, version 6.8. The simulation utilized a single finite element C3D8H7. It has been assumed that the material is almost ideally incompressible.

The displacement vector components at each of the nodes have been displayed in Figure 4. The \(i\)-th \((i = 1, 2, 3)\) displacement vector component at \(j\)-th \((j = 1, 2, \ldots, 8)\) node has been denoted as \(u_{ij}\). The \(u_{ij}\) displacement components (direction „1“) have been set to \(\Delta u\) for the nodes 5, 6, 7 and 8, whereas some displacements have been fixed to equal zero in order to exclude the possibility of rigid body motion. The employed set of boundary conditions allowed for obtaining the state of uniaxial tension in the entire volume of the finite element. Due to the assumed incompressibility the deformation gradient corresponding to the given deformation process takes the form:

\[\begin{align*}
DDSDDE(3, 4) &= \text{TWO}/\text{THREE} \ast \text{TERM1} \ast \text{BBAR}(4) + \text{TERM2} \ast \text{BBAR}(3) - \text{TRBBAR} \ast \text{BBAR}(4) \\
DDSDDE(4, 4) &= \text{ONE}/\text{TWO} \ast \text{TERM1} \ast (\text{BBAR}(1) + \text{BBAR}(2)) \\
\text{IF} (\text{NSHR} = 3) \text{ THEN} \\
DDSDDE(1, 5) &= \text{ONE}/\text{THREE} \ast \text{TERM1} \ast \text{BBAR}(5) + \text{TERM2} \ast (\text{BBAR}(1) - \text{TRBBAR}) \ast \text{BBAR}(5) \\
DDSDDE(2, 5) &= -\text{TWO}/\text{THREE} \ast \text{TERM1} \ast \text{BBAR}(5) + \text{TERM2} \ast (\text{BBAR}(2) - \text{TRBBAR}) \ast \text{BBAR}(5) \\
DDSDDE(3, 5) &= \text{ONE}/\text{THREE} \ast \text{TERM1} \ast \text{BBAR}(5) + \text{TERM2} \ast (\text{BBAR}(3) - \text{TRBBAR}) \ast \text{BBAR}(5) \\
\text{IF} (\text{NSHR} = 3) \text{ THEN} \\
DDSDDE(1, 6) &= -\text{TWO}/\text{THREE} \ast \text{TERM1} \ast \text{BBAR}(6) + \text{TERM2} \ast (\text{BBAR}(1) - \text{TRBBAR}) \ast \text{BBAR}(6) \\
DDSDDE(2, 6) &= \text{ONE}/\text{THREE} \ast \text{TERM1} \ast \text{BBAR}(6) + \text{TERM2} \ast (\text{BBAR}(2) - \text{TRBBAR}) \ast \text{BBAR}(6) \\
DDSDDE(3, 6) &= \text{ONE}/\text{THREE} \ast \text{TERM1} \ast \text{BBAR}(6) + \text{TERM2} \ast (\text{BBAR}(3) - \text{TRBBAR}) \ast \text{BBAR}(6) \\
\text{IF} (\text{NSHR} = 3) \text{ THEN} \\
DDSDDE(5, 5) &= \text{ONE}/\text{TWO} \ast \text{TERM1} \ast (\text{BBAR}(3) + \text{BBAR}(1)) + \\
\text{TERM2} \ast \text{BBAR}(5) \ast \text{TWO} \\
DDSDDE(6, 6) &= \text{ONE}/\text{TWO} \ast \text{TERM1} \ast (\text{BBAR}(3) + \text{BBAR}(2)) + \\
\text{TERM2} \ast \text{BBAR}(6) \ast \text{TWO} \\
DDSDDE(4, 5) &= \text{ONE}/\text{TWO} \ast \text{TERM1} \ast \text{BBAR}(6) + \text{TERM2} \ast ((\text{BBAR}(4) + \text{BBAR}(5) - \text{TRBBAR}) \ast \text{BBAR}(6) \\
DDSDDE(4, 6) &= \text{ONE}/\text{TWO} \ast \text{TERM1} \ast \text{BBAR}(5) + \text{TERM2} \ast ((\text{BBAR}(4) + \text{BBAR}(5) - \text{TRBBAR}) \ast \text{BBAR}(6) \\
DDSDDE(5, 6) &= \text{ONE}/\text{TWO} \ast \text{TERM1} \ast \text{BBAR}(4) + \text{TERM2} \ast ((\text{BBAR}(5) + \text{BBAR}(6) - \text{TRBBAR}) \ast \text{BBAR}(6) \\
\text{END IF} \\
\text{DO K1=1, NTENS} \\
\text{DO K2=1, K1-1} \\
\text{DDSDDE(K1, K2)=DDSDDE(K2, K1)} \\
\text{END DO} \\
\text{END DO} \\
\text{RETURN} \\
\text{END}
\end{align*}\]

\[^7\] cubic, three-dimensional, 8 nodes, hybrid.
where $\lambda_1$ denotes the stretch ratio in the direction “1”.

The data obtained from a uniaxial tension test performed on high density polyethylene (HDPE) [7] at the deformation rate of $0.004 \, s^{-1}$ [7] were used to determine the constants $\mu$, $b$ and $n$. The inverse of the bulk modulus $D_1$ has been set to $0.000000033 \, MPa^{-1}$ in order to account for almost incompressible deformation. In Figure 5 the theoretical predictions of the FEM
simulation have been compared to the experimental data. It can be seen that the agreement is very good. The described simulation has been repeated for greater number of finite elements without any difference in results.

7. Conclusions

This paper presents the full way of derivation of an analytical elasticity tensor characterizing the mechanical behavior of a hyperelastic material. The described framework is valid for both isotropic and anisotropic hyperelastic materials. The analytical elasticity tensor associated with the Knowles hyperelastic model has been derived and presented for the first time in the literature.

Basing on the derived elasticity tensor, a FORTRAN code has been written, allowing for the implementation of the Knowles material model into the FEA system Abaqus. The agreement between the experimental and FEM predictions is very good (Fig. 5.). The code has been presented in the work and is ready to use. Since the code is based on an analytical elasticity tensor, it guarantees quadratic convergence for all kinds of boundary value problems of nonlinear elasticity.

As it has been pointed out at the beginning of the text, the Knowles material model, although not very popular, is probably the most effective potential function, when it comes to modeling of the nonlinear elasticity of thermoplastics, polymeric composites and some of the biological tissues such as bone for instance. It is possible to develop more sophisticated models which take into account such behaviors as viscoelasticity, plasticity, strain rate dependency, hysteresis and other. Since the analytical elasticity tensor is available now, the advanced models do not have to be based on the theories offered by the commercial FEA systems.

A. Derivation of constitutive rate equation

By taking a material time derivative of (6) one can obtain a rate form of the constitutive equation describing a hyperelastic material:

\[
\dot{S} = 4 \frac{\partial^2 W_e}{\partial C \partial \dot{C}} \cdot \frac{1}{2} \dot{\mathbf{C}} = \mathbf{C} \cdot \frac{1}{2} \dot{\mathbf{C}}
\]  

(28)

where \( \mathbf{C} \) is the elasticity tensor expressed by means of the Lagrangian variables.
As it will be shown below, the constitutive rate equation given by (28) can be transformed into the current configuration and take the form which is typical for hypoelastic constitutive relations\(^8\).

For the sake of the further derivations, the following relations are needed:

\[
\dot{C} = \dot{F}^T F + F^T \dot{F}, \quad L = \dot{F} F^{-1} = -\dot{F} F^{-1}, \quad S = F^{-1} \tau F^{-T},
\]

\[
\dot{S} = \dot{F}^{-1} \tau F^{-T} + F^{-1} \dot{\tau} F^{-T} + F^{-1} \tau \dot{F}^{-T}.
\]

The last of the equations given above follows from taking a material time derivative of the transformation law \(S = F^{-1} \tau F^{-T}\).

By substituting the first and the last of the given above relations into (28), it is found that:

\[
F^{-1} \dot{\tau} F^{-T} + F^{-1} \tau F^{-T} + F^{-1} \tau \dot{F}^{-T} = \mathbf{C} \cdot \frac{1}{2} (\dot{F}^T F + F^T \dot{F})
\]

(29)

Right-multiplying of (29) by \(F\) and left-multiplying by \(F^T\) results in:

\[
\dot{\tau} + \dot{F} F^{-1} \tau + \tau \dot{F}^{-T} F^T = F \left\{ \mathbf{C} \cdot \frac{1}{2} (\dot{F}^T F + F^T \dot{F}) \right\} F^T
\]

or equivalently

\[
\dot{\tau} + \dot{F} F^{-1} \tau + \tau \left( F F^{-1} \right)^T = F \left\{ \mathbf{C} \cdot \frac{1}{2} F^T \left( F^{-T} \dot{F}^T + \dot{F} F^{-1} \right) F \right\} F^T
\]

or

\[
\dot{\tau} + \dot{F} F^{-1} \tau + \tau \left( F F^{-1} \right)^T = F \left\{ \mathbf{C} \cdot \frac{1}{2} F^T \left( (F F^{-1})^T + \dot{F} F^{-1} \right) F \right\} F^T.
\]

By making use of the definition of strain rate tensor, namely \(D = \frac{1}{2} (L^T + L)\) and recalling the given above definition of the velocity gradient, it is found that:

\[
\dot{\tau} - L \tau - \tau L^T = F \left\{ \mathbf{C} \cdot (F^T DF) \right\} F^T.
\]

---

\(^8\) Generally, hypoelasticity, elasticity and hyperelasticity are not equivalent. However it has been proved by Noll that for some special cases it is possible to transform a hypoelastic constitutive relation into an elastic constitutive relation [8]. It should be noticed that a hyperelastic material is an elastic material which possesses a stored-energy potential. Thus, there is a link between the hypoelastic and hyperelastic constitutive relations. Every hyperelastic constitutive relation can be transformed into a hypoelastic constitutive relation and the current section describes the general framework of the transformation. It is important that the rule stated above is not reversible. Only some of the hypoelastic constitutive relations can be transformed into the form of hyperelastic relations.
The components of the expression on the right side of (30) are given by the formula:

\[
\left\{ F \left[ \mathcal{C} \cdot (F^T \mathbf{D} F) \right] \right\}_{ij} = C_{pqrs} F_{ip} F_{jq} F_{kr} F_{ls} D_{kl}. \tag{31}
\]

A new, transformed elasticity tensor \( \mathcal{C}^{rc} \) can be introduced. Its components are defined as follows:

\[
C_{ijkl}^{rc} = C_{pqrs} F_{ip} F_{jq} F_{kr} F_{ls}. \tag{32}
\]

Thus, (30) takes the form:

\[
\dot{\tau} - L\tau - \tau L^T = \mathcal{C}^{rc} \cdot \mathbf{D} \tag{33}
\]

where \( L\tau = \dot{\tau} - L\tau - \tau L^T \) defines convected objective rate of the Kirchhoff stress \( \tau \). By taking into account the fact that \( L = D + W \) and introducing new fourth order tensor \( H \), it is found that:

\[
\dot{\tau} - W\tau - \tau W^T = \mathcal{C}^{rc} \cdot \mathbf{D} + \mathbf{D}\tau + \tau \mathbf{D}^T \tag{34}
\]

where the components of \( H \) are given by the following formula:

\[
(H)_{ijkl} = \frac{1}{2} \left( \delta_{ik} \tau_{jl} + \tau_{ik} \delta_{jl} + \delta_{il} \tau_{jk} + \tau_{il} \delta_{jk} \right). \tag{35}
\]

Finally, a rate form of the constitutive equation using the Zaremba-Jaumann objective rate is obtained:

\[
\dot{\tau} - W\tau - \tau W^T = \mathcal{C}^{Z-J} \cdot \mathbf{D} \tag{36}
\]

where \( \mathcal{C}^{Z-J} = \mathcal{C}^{rc} + H \) is a new elasticity tensor associated to the Zaremba-Jaumann objective rate of the Kirchhoff stress, namely \( \tau^\prime = \dot{\tau} - W\tau - \tau W^T \).

**B. Derivation of elasticity tensor in general form**

The uncoupled form of the stored-energy function \( W_e \), as stated before, is given by the following equation:

\[
W_e(C) = U(J) + \overline{W}(\overline{C}) \tag{37}
\]

where \( U(J) \) and \( \overline{W}(\overline{C}) \) denote volumetric and isochoric component, respectively. By substituting (37) into the general form of the constitutive equation given by (6), it can be found that:

\[
\mathbf{S} = J \frac{\partial U}{\partial J} \mathbf{C}^{-1} + 2J^{-2/3} \left[ \frac{\partial \overline{W}}{\partial \overline{C}} - \frac{1}{3} \left( \frac{\partial \overline{W}}{\partial \overline{C}} \cdot \overline{C} \right) \overline{C}^{-1} \right] \tag{38}
\]
which is the general form of the constitutive equation with uncoupled volumetric and isochoric components.

The material elasticity tensor is defined by the formula:

\[ C = 2 \frac{\partial S}{\partial C} = 4 \frac{\partial^2 W_e}{\partial C \partial C}. \]  

(39)

The substitution of (38) into (39) and systematic use of the chain rule leads by turns to the following results:

\[
C = 2 \frac{\partial S}{\partial C} = 2 \frac{\partial}{\partial C} \left( 2 \frac{\partial W_e}{\partial C} \right) \\
= 2 \frac{\partial}{\partial C} \left( J \frac{\partial U}{\partial J} C^{-1} + 2 J^{-2/3} \left[ \frac{\partial W}{\partial C} - \frac{1}{3} \left( \frac{\partial W}{\partial C} \cdot C \right) C^{-1} \right] \right) \\
= 2 \frac{\partial}{\partial C} \left( J \frac{\partial U}{\partial J} C^{-1} \right) + 2 \frac{\partial}{\partial C} \left( 2 J^{-2/3} \left[ \frac{\partial W}{\partial C} - \frac{1}{3} \left( \frac{\partial W}{\partial C} \cdot C \right) C^{-1} \right] \right) \\
= 2 \frac{\partial U}{\partial J} C^{-1} \otimes \frac{\partial J}{\partial C} + 2 J \frac{\partial U}{\partial J} C^{-1} \otimes \frac{\partial}{\partial C} \left( \frac{\partial U}{\partial J} \right) \\
+ 4 \left[ \frac{\partial W}{\partial C} - \frac{1}{3} \left( \frac{\partial W}{\partial C} \cdot C \right) C^{-1} \right] \otimes \frac{\partial J^{-2/3}}{\partial C} \\
+ 4 J^{-2/3} \frac{\partial}{\partial C} \left[ \frac{\partial W}{\partial C} - \frac{1}{3} \left( \frac{\partial W}{\partial C} \cdot C \right) C^{-1} \right] \otimes \frac{\partial J}{\partial C} \\
= 2 \frac{\partial U}{\partial J} C^{-1} \otimes \frac{\partial J}{\partial C} + 2 J \frac{\partial U}{\partial J} C^{-1} \otimes \frac{\partial}{\partial C} \frac{\partial U}{\partial J} \\
- \frac{8}{3} J^{-5/3} \left[ \frac{\partial W}{\partial C} - \frac{1}{3} \left( \frac{\partial W}{\partial C} \cdot C \right) C^{-1} \right] \otimes \frac{\partial J}{\partial C} \\
+ 4 J^{-2/3} \left[ \frac{\partial^2 W}{\partial C \partial C} \cdot C^{-1} - \frac{1}{3} C^{-1} \otimes \frac{\partial}{\partial C} \left( \frac{\partial W}{\partial C} \cdot C \right) - \frac{1}{3} \left( \frac{\partial W}{\partial C} \cdot C \right) \frac{\partial C^{-1}}{\partial C} \right].
\]

For the use of further derivations the following relations are needed:

\[
\frac{\partial J}{\partial C} = \frac{1}{2} J C^{-1}, \quad \frac{\partial C^{-1}}{\partial C} = -I C^{-1}, \quad \frac{\partial C}{\partial C} = J^{-2/3} \left( I - \frac{1}{3} C \otimes C^{-1} \right), \\
\frac{\partial C^{-1}}{\partial C} = J^{-2/3} \left( \frac{1}{3} C^{-1} \otimes C^{-1} - J^{4/3} I C^{-1} \right).
\]
The given relations allow to calculate the necessary terms as shown below:

\[
\begin{align*}
\frac{\partial^2 W}{\partial \mathbf{C} \partial \mathbf{C}} \cdot \frac{\partial \mathbf{C}}{\partial \mathbf{C}} &= J^{-2/3} \frac{\partial^2 W}{\partial \mathbf{C} \partial \mathbf{C}} \cdot \left( \mathbf{I} - \frac{1}{3} \mathbf{C} \otimes \mathbf{C}^{-1} \right) \\
&= J^{-2/3} \frac{\partial^2 W}{\partial \mathbf{C} \partial \mathbf{C}} - \frac{1}{3} J^{-2/3} \left( \frac{\partial^2 W}{\partial \mathbf{C} \partial \mathbf{C}} \cdot \mathbf{C}^{-1} \right) \otimes \mathbf{C}^{-1},
\end{align*}
\]

(40)

\[
\begin{align*}
\frac{\partial}{\partial \mathbf{C}} \left( \frac{\partial W}{\partial \mathbf{C}} \cdot \mathbf{C}^{-1} \right) &= \mathbf{C} \cdot \frac{\partial^2 W}{\partial \mathbf{C} \partial \mathbf{C}} \cdot \frac{\partial \mathbf{C}}{\partial \mathbf{C}} + \frac{\partial W}{\partial \mathbf{C}} \cdot \frac{\partial \mathbf{C}}{\partial \mathbf{C}} \\
&= J^{-2/3} \mathbf{C} \cdot \frac{\partial^2 W}{\partial \mathbf{C} \partial \mathbf{C}} \cdot \left( \mathbf{I} - \frac{1}{3} \mathbf{C} \otimes \mathbf{C}^{-1} \right) \\
&+ J^{-2/3} \frac{\partial W}{\partial \mathbf{C}} \cdot \left( \mathbf{I} - \frac{1}{3} \mathbf{C} \otimes \mathbf{C}^{-1} \right) \\
&= J^{-2/3} \left( \mathbf{C} \cdot \frac{\partial^2 W}{\partial \mathbf{C} \partial \mathbf{C}} \right) \\
&- \frac{1}{3} J^{-2/3} \left( \mathbf{C} \cdot \frac{\partial^2 W}{\partial \mathbf{C} \partial \mathbf{C}} \cdot \mathbf{C}^{-1} \right) \otimes \mathbf{C}^{-1} \\
&+ J^{-2/3} \frac{\partial W}{\partial \mathbf{C}} \cdot \frac{\partial \mathbf{C}}{\partial \mathbf{C}}
\end{align*}
\]

(41)

and finally

\[
\frac{\partial \mathbf{C}^{-1}}{\partial \mathbf{C}} = J^{-2/3} \left( \frac{1}{3} \mathbf{C}^{-1} \otimes \mathbf{C}^{-1} - J^{4/3} \mathbf{I}_{\mathbf{C}^{-1}} \right).
\]

(42)

Using the results given above in the equation expressing the elasticity tensor, we obtain the final formula:

\[
\mathbf{C} = J \frac{\partial \mathbf{U}}{\partial \mathbf{J}} \left( \mathbf{C}^{-1} \otimes \mathbf{C}^{-1} - 2 \mathbf{I}_{\mathbf{C}^{-1}} \right) + J^2 \frac{\partial^2 \mathbf{U}}{\partial \mathbf{J}^2} \mathbf{C}^{-1} \otimes \mathbf{C}^{-1}
\]

\[
- \frac{4}{3} J^{-4/3} \left( \frac{\partial \mathbf{W}}{\partial \mathbf{C}} \otimes \mathbf{C}^{-1} + \mathbf{C}^{-1} \otimes \frac{\partial \mathbf{W}}{\partial \mathbf{C}} \right)
\]

\[
+ \frac{4}{3} J^{-4/3} \left( \frac{\partial \mathbf{W}}{\partial \mathbf{C}} \cdot \mathbf{C}^{-1} \right) \left( J^{4/3} \mathbf{I}_{\mathbf{C}^{-1}} + \frac{1}{3} \mathbf{C}^{-1} \otimes \mathbf{C}^{-1} \right) + J^{-4/3} \mathbf{C}_W
\]

where

\[
\mathbf{C}_W = 4 \frac{\partial^2 \mathbf{W}}{\partial \mathbf{C} \partial \mathbf{C}} - \frac{4}{3} \left[ \left( \frac{\partial^2 \mathbf{W}}{\partial \mathbf{C} \partial \mathbf{C}} \cdot \mathbf{C}^{-1} \right) \otimes \mathbf{C}^{-1} + \mathbf{C}^{-1} \otimes \left( \mathbf{C} \cdot \frac{\partial^2 \mathbf{W}}{\partial \mathbf{C} \partial \mathbf{C}} \right) \right]
\]

\[
+ \frac{4}{9} \left( \mathbf{C} \cdot \frac{\partial^2 \mathbf{W}}{\partial \mathbf{C} \partial \mathbf{C}} \right) \mathbf{C}^{-1} \otimes \mathbf{C}^{-1}.
\]

(44)
C. Derivation of elasticity tensor associated to Knowles material

For the use of FEM implementation the Knowles stored-energy function is decoupled into an isochoric and a volumetric components. The definition of the isochoric component corresponds to the definition of the Knowles stored-energy function [11], namely:

$$ W = \frac{\mu}{2b} \left\{ \left( 1 + \frac{b}{n} (I_1 - 3) \right)^n - 1 \right\}. \quad (45) $$

The simplest possible form of the volumetric component has been chosen:

$$ U = \frac{1}{D_1} (J - 1)^2. \quad (46) $$

According to (43) and (44), the following derivatives have to be calculated in order to find an expression for the elasticity tensor:

$$ \frac{\partial W}{\partial I_1} = \frac{\mu}{2} \left[ 1 + \frac{b}{n} (I_1 - 3) \right]^{n-1}, \quad (47) $$

$$ \frac{\partial W}{\partial C} = \frac{\partial W}{\partial I_1} 1 = \frac{\mu}{2} \left[ 1 + \frac{b}{n} (I_1 - 3) \right]^{n-1} 1, \quad (48) $$

$$ \frac{\partial U}{\partial J} = \frac{2}{D_1} (J - 1), \quad \frac{\partial^2 U}{\partial J^2} = \frac{2}{D_1}. \quad (49) $$

The second derivatives are more difficult to calculate. They are obtained by a systematic use of the chain rule:

$$ \frac{\partial^2 W}{\partial C \partial C} = \frac{\partial}{\partial C} \left( \frac{\partial W}{\partial C} \right) $$

$$ = \frac{\partial}{\partial C} \left( \frac{\partial W}{\partial I_1} 1 \right) $$

$$ = \frac{\partial}{\partial C} \left[ \frac{\partial W}{\partial I_1} \right] $$

$$ = 1 \otimes \frac{\partial}{\partial C} \left( \frac{\partial W}{\partial I_1} \right) $$

$$ = 1 \otimes \left\{ \frac{\partial}{\partial I_1} \left( \frac{\mu}{2} \left[ 1 + \frac{b}{n} (I_1 - 3) \right]^{n-1} \right) \frac{\partial I_1}{\partial C} \right\} $$

$$ = 1 \otimes \left\{ \frac{\mu b(n-1)}{2n} \left[ 1 + \frac{b}{n} (I_1 - 3) \right]^{n-2} \right\} 1 $$

$$ = \frac{\mu b(n-1)}{2n} \left[ 1 + \frac{b}{n} (I_1 - 3) \right]^{n-2} 1 \otimes 1. \quad (50) $$
What is more the following expressions are needed:

\[
\left( \frac{\partial W}{\partial \mathbf{C}} \cdot \mathbf{C} \right) = \frac{\mu}{2} \left[ 1 + \frac{b}{n} (\bar{I}_1 - 3) \right]^{n-1} (1 \cdot \mathbf{C}) \tag{51}
\]

\[
\left( \frac{\partial^2 W}{\partial \mathbf{C} \partial \mathbf{C}} \cdot \mathbf{C} \right) = \frac{\mu b(n-1)}{2} \left[ 1 + \frac{b}{n} (\bar{I}_1 - 3) \right]^{n-2} (1 \cdot \mathbf{C}) \mathbf{1} \tag{52}
\]

\[
\left( \mathbf{C} \cdot \frac{\partial^2 W}{\partial \mathbf{C} \partial \mathbf{C}} \cdot \mathbf{C} \right) = \frac{\mu b(n-1)}{2} \left[ 1 + \frac{b}{n} (\bar{I}_1 - 3) \right]^{n-2} (\mathbf{C} \cdot \mathbf{1}) (1 \cdot \mathbf{C}) \tag{53}
\]

\[
\left( \mathbf{C} \cdot \frac{\partial^2 W}{\partial \mathbf{C} \partial \mathbf{C}} \cdot \mathbf{C} \right) = \frac{\mu b(n-1)}{2} \left[ 1 + \frac{b}{n} (\bar{I}_1 - 3) \right]^{n-2} (\mathbf{C} \cdot \mathbf{1}) (1 \cdot \mathbf{C}) \tag{54}
\]

Substituting (48), (49), (50), (51), (52), (53), and (54), into (43) and (44) results in the following formula for the elasticity tensor corresponding to the Knowles stored-energy function:

\[
\mathbf{C} = \frac{2}{D_1} J (J - 1) (\mathbf{C}^{-1} \otimes \mathbf{C}^{-1} - 2 \mathbf{I}_{\mathbf{C}^{-1}}) + J^2 \frac{2}{D_1} \mathbf{C}^{-1} \otimes \mathbf{C}^{-1}
\]

\[
- \frac{2}{3} J^{-2/3} \mu \left[ 1 + \frac{b}{n} (\bar{I}_1 - 3) \right]^{n-1} \left( \mathbf{1} \otimes \mathbf{C}^{-1} + \mathbf{C}^{-1} \otimes \mathbf{1} \right)
\]

\[
+ \frac{2}{3} \mu \left[ 1 + \frac{b}{n} (\bar{I}_1 - 3) \right]^{n-1} \bar{I}_1 \left( \mathbf{1}_{\mathbf{C}^{-1}} + \frac{1}{3} \mathbf{C}^{-1} \otimes \mathbf{C}^{-1} \right)
\]

\[
+ 2 J^{-4/3} \mu \frac{b(n-1)}{n} \left[ 1 + \frac{b}{n} (\bar{I}_1 - 3) \right]^{n-2} \mathbf{1} \otimes \mathbf{1}
\]

\[
- \frac{2}{3} J^{-2/3} \mu \frac{b(n-1)}{n} \left[ 1 + \frac{b}{n} (\bar{I}_1 - 3) \right]^{n-2} \bar{I}_1 \left( \mathbf{1} \otimes \mathbf{C}^{-1} + \mathbf{C}^{-1} \otimes \mathbf{1} \right)
\]

\[
+ \frac{2}{9} \mu \frac{b(n-1)}{n} \left[ 1 + \frac{b}{n} (\bar{I}_1 - 3) \right]^{n-2} \bar{I}_1^2 \mathbf{C}^{-1} \otimes \mathbf{C}^{-1}
\]
The elasticity tensor associated to the convected rate of the Kirchhoff stress is obtained by the use of the transformation rule $C_{ijkl}^{rc} = F_{ip}F_{jq}F_{kr}F_{ls}C_{pqrs}$.

It takes the form:

$$C_{ijkl}^{rc} = \frac{2}{D_1} J(J - 1) (1 \otimes 1 - 2I) + J^2 \frac{2}{D_1} 1 \otimes 1 - \frac{2}{3} J^{-2/3} \mu \left[ 1 + \frac{b}{n} (\overline{I}_1 - 3) \right]^{n-1} (B \otimes 1 + 1 \otimes B) + \frac{2}{3} \mu \left[ 1 + \frac{b}{n} (\overline{I}_1 - 3) \right]^{n-1} \overline{I}_1 \left( I + \frac{1}{3} 1 \otimes 1 \right) + 2 J^{-4/3} \mu \frac{b(n - 1)}{n} \left[ 1 + \frac{b}{n} (\overline{I}_1 - 3) \right]^{n-2} B \otimes B - \frac{2}{3} J^{-2/3} \mu \frac{b(n - 1)}{n} \left[ 1 + \frac{b}{n} (\overline{I}_1 - 3) \right]^{n-1} \overline{I}_1 (B \otimes 1 + 1 \otimes B) + \frac{2}{9} \mu \frac{b(n - 1)}{n} \left[ 1 + \frac{b}{n} (\overline{I}_1 - 3) \right]^{n-2} \overline{I}_1^2 1 \otimes 1. \quad (56)$$

The substitution of (48) and (49) into (38) gives the following form of the constitutive equation in the reference configuration:

$$S = \frac{2}{D_1} J(J - 1) C^{-1} + \mu \left[ 1 + \frac{b}{n} (\overline{I}_1 - 3) \right]^{n-1} \left( J^{-2/3} 1 - \frac{1}{3} \overline{I}_1 C^{-1} \right). \quad (57)$$

Using the transformation rule $\tau = FSF^T$ results in a formula for the Kirchhoff stress:

$$\tau = \frac{2}{D_1} J(J - 1) 1 + \mu \left[ 1 + \frac{b}{n} (\overline{I}_1 - 3) \right]^{n-1} \left( B - \frac{1}{3} \overline{I}_1 1 \right). \quad (58)$$

Making use of the relation:

$$C_{ijkl}^{rc} = C_{ijkl}^{rc} + \frac{1}{2} \left( \delta_{ik} \tau_{jl} + \tau_{ik} \delta_{jl} + \delta_{il} \tau_{jk} + \tau_{il} \delta_{jk} \right) e_i \otimes e_j \otimes e_k \otimes e_l \quad (59)$$
By substituting (60) into the equation

\[ C^{\tau Z-J}_{ijkl} = \frac{2}{D_1} J (J - 1) \left( \delta_{ij} \delta_{kl} - \delta_{ik} \delta_{jl} - \delta_{il} \delta_{jk} \right) + \frac{2}{D_1} J^2 \delta_{ij} \delta_{kl} \]

\[ + \frac{2}{3} \mu \left[ 1 + \frac{b}{n} \left( \bar{I}_1 - 3 \right) \right]^{n-1} \left[ \bar{I}_1 \left( \frac{1}{2} \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) + \frac{1}{3} \delta_{ij} \delta_{kl} \right) \right] \]

\[ - \frac{1}{3} \bar{I}_1 \left( \bar{B}_{ij} \delta_{kl} - \bar{B}_{ij} \bar{B}_{kl} \right) + \frac{1}{9} \bar{I}_1 \delta_{ij} \delta_{kl} + \frac{1}{9} \bar{I}_1 \delta_{ij} \delta_{kl} \]

\[ + \frac{1}{D_1} J (J - 1) \delta_{ik} \delta_{jl} + \frac{\mu}{2} \left[ 1 + \frac{b}{n} \left( \bar{I}_1 - 3 \right) \right]^{n-1} \left( \delta_{ik} \bar{B}_{jl} - \frac{1}{3} \bar{I}_1 \delta_{ik} \delta_{jl} \right) \]

After simplifying the above relation, the following expression for the elasticity tensor associated to the Zaremba-Jaumann objective rate of the Kirchhoff stress is obtained:

\[ C^{\tau Z-J}_{ijkl} = \mu \left[ 1 + \frac{b}{n} \left( \bar{I}_1 - 3 \right) \right]^{n-1} \left[ \frac{1}{2} \left( \delta_{ik} \bar{B}_{jl} + \delta_{jl} \bar{B}_{ik} \right. \right. \]

\[ + \delta_{il} \bar{B}_{jk} + \delta_{jk} \bar{B}_{il} \left. \right] + \frac{2}{3} \left[ 1 + \frac{b}{n} \left( \bar{I}_1 - 3 \right) \right]^{n-2} \bar{B}_{ij} \bar{B}_{kl} - \frac{1}{3} \bar{I}_1 \left( \bar{B}_{ij} \delta_{kl} \right) \]

\[ + 2 \mu \left( \frac{b(n - 1)}{n} \right) \left[ 1 + \frac{b}{n} \left( \bar{I}_1 - 3 \right) \right]^{n-2} \left( \bar{B}_{ij} \delta_{kl} - \frac{1}{3} \bar{I}_1 \delta_{ij} \delta_{kl} \right) \]

\[ + \frac{1}{9} \bar{I}_1 \delta_{ij} \delta_{kl} \right] \]

\[ \frac{2}{D_1} J (2J - 1) \delta_{ij} \delta_{kl} \] (60)

By substituting (60) into the equation

\[ C^{MZ-J}_{ijkl} = \frac{1}{J} C^{\tau Z-J}_{ijkl} \] (61)
the form of the elasticity tensor accepted by Abaqus is found:

\[
C_{ijkl}^{MKZ-J} = \frac{\mu}{J} \left[ 1 + \frac{b}{n} (\bar{I}_1 - 3) \right]^{n-1} \left[ \frac{1}{2} (\delta_{ik} \bar{B}_{jl} + \delta_{jl} \bar{B}_{ik}) + \delta_{il} \bar{B}_{jk} + \delta_{jk} \bar{B}_{il} + \frac{2}{3} \left( \frac{1}{3} \bar{I}_1 \delta_{ij} \delta_{kl} - \bar{B}_{ij} \delta_{kl} - \delta_{ij} \bar{B}_{kl} \right) \right] + \frac{2 \mu b(n - 1)}{J} \left[ 1 + \frac{b}{n} (\bar{I}_1 - 3) \right]^{n-2} \left[ \bar{B}_{ij} \bar{B}_{kl} - \frac{1}{3} \bar{I}_1 \bar{B}_{ij} \delta_{kl} \right] + \delta_{ij} \bar{B}_{kl},
\]

(62)

It can be noticed that for \( b = 1 \) and \( n = 1 \) the elasticity tensor corresponding to the Knowles stored-energy tensor reduces to the elasticity tensor of Neo-Hooke hyperelastic model.

REFERENCES

Wprowadzenie funkcji energii potencjalnej typu Knowlesa do systemu metody elementów skończonych: teoria, kodowanie i zastosowania

Streszczenie

Praca przedstawia pełną drogę wprowadzania do systemu metody elementów skończonych (MES) równania konstytutywnego hipersprężystości zdefiniowanego przez użytkownika przy użyciu odpowiedniego tensora sztywności. Aby zilustrować metodykę wprowadzania równania konstytutywnego do MES posłużono się modelem materiału hipersprężystego typu Knowlesa, gdyż model ten dobrze opisuje nieliniową sprężystość w zakresie średnich deformacji. Stąd model Knowlesa pozwala na poprawne zdefiniowanie własności mechanicznych polimerów termoplastycznych, żywic, kompozytów polimerowych oraz niektórych tkanek biologicznych, jak np. tkanka kostna. Przedstawiono podział równania konstytutywnego na część izochoryczną i objętościową. Wyprowadzono analitycznie tensor sztywności odpowiadający modelowi Knowlesa. Zdefiniowany tensor sztywności może dalej posłużyć do budowy równań konstytutywnych nieliniowej lepkosprężystości lub lepkoplastyczności. W celu wprowadzenia modelu do systemu MES napisany został program w języku FORTRAN 77. W pracy przedstawiono wyniki z prostej symulacji MES wykonanej ze względu na wcześniejsze opisane zastosowania.