A comparison of three non-linear constitutive models

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P.M. van Kemenade

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Coaches: Prof. Dr. Ir. J.D. Janssen
Dr. Ir. C.W.J. Oomens
Ir. O.M.G.C. op den Camp

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Chapter 1

Constitutive laws

1.1 Introduction

In this chapter three constitutive models will be analyzed. The models are in literature given by strain-energy functions. In the first section the relation between the strain-energy function and the 2nd Piola-Kirchhoff stress tensor is given. With this relation the 2nd Piola-Kirchhoff stress tensors for the three models are derived.

In the next section two simple test problems, uniaxial stretch and simple shear are worked out using the three models. In the last section the plane stress situation is given for each model.

1.2 The strain-energy function

With the second law of thermodynamics, it is possible to derive that the 2nd Piola-Kirchhoff stress tensor can be related to the free energy. The stress-deformation relation is simply:

$$\mathcal{P}\,(,\mathcal{S}) = \rho_0 \frac{\partial \psi(\mathcal{E})}{\partial \mathcal{E}} = \rho_0 \frac{\partial \psi(\mathcal{C})}{\partial \mathcal{C}} : \frac{\partial \mathcal{C}}{\partial \mathcal{E}} = 2\rho_0 \frac{\partial \psi(\mathcal{C})}{\partial \mathcal{C}} \tag{1.1}$$

where:
$\mathcal{P}$ = 2nd Piola-Kirchhoff stress tensor
$\mathcal{S}$ = 2nd Piola-Kirchhoff stress tensor based on the deviatoric stress
ρ_0= mass density
ψ= free energy
$\mathcal{E}$=Green Lagrange strain tensor
$\mathcal{C}$=Cauchy Green strain tensor

W=$\rho_0\,\psi$ is an elastic potential energy function (also called the strain-energy function). The stress-deformation relation becomes:

$$\mathcal{P}\,(,\mathcal{S}) = \frac{\partial W(\mathcal{E})}{\partial \mathcal{E}} = 2\,\frac{\partial W(\mathcal{C})}{\partial \mathcal{C}} \tag{1.2}$$

In the next subsections these relations are used to determine the 2nd Piola Kirchoff stress tensors from three different strain energy functions.

1.2.1 Strain-energy function by Mow/Holmes

The strain-energy function used by Mow/Holmes [1] to describe the non linear isotropic characteristics of soft gels and hydrated tissues in ultrafiltration yields:

$$\rho_0\, \psi(\mathcal{C}) = W(\mathcal{C}) = \alpha_0\, \frac{exp\,(\alpha_1\,(J_1 - 3) + \alpha_2\,(J_2 - 3))}{{J_3}^{\beta}} \tag{1.3}$$

where:
ψ = free-energy
W = strain-energy function
ρ_0 = mass density
$\alpha_0, \alpha_1, \alpha_2$= positive constants
$\beta = \alpha_1 + 2\alpha_2$
J_1, J_2, J_3 = three principal invariants of the Cauchy Green strain tensor

Using equation 1.2 it is possible to determine the second Piola-Kirchhoff stress tensor. (Appendix A)

$$\mathcal{P} = 2W\{(\alpha_1 + \alpha_2 J_1 - \frac{J_2}{J_3}\,\beta)\,\mathcal{I} + (-\alpha_2 + \frac{J_1}{J_3}\,\beta)\mathcal{C} - \frac{\beta}{J_3}\,\mathcal{C}^2\} \tag{1.4}$$

1.2.2 Strain-energy function by Bovendeerd

Bovendeerd [2] uses the following strain-energy function to describe the mechanical behaviour of the passive (heart) myocardium (transversely isotropic with respect to the $\vec{e}_3$-direction).

$$W(\mathcal{E}) = c\,[exp\,(a_1 {I_E}^2 + a_2 II_E + a_3 {E_{33}}^2 + a_4({E_{31}}^2 + {E_{32}}^2)) - 1] \tag{1.5}$$

where:
c, a_1, a_2, a_3, a_4 = material parameters
$I_E = E_{11} + E_{22} + E_{33} = J_1$
$II_E = E_{12}^2 + E_{23}^2 + E_{31}^2 - E_{11}E_{22} - E_{22}E_{33} - E_{33}E_{11} = -J_2$
J_1, J_2 = principal invariants of the Green-Lagrange strain tensor

Because of the incompressibility of the cardiac tissue, the scalar $III_E = \det(\mathcal{E})$ is left out of this strain-energy function.

Equation 1.2 supposes that W is symmetrized in the variables E_{ij} and E_{ji}. If this is not the case, the symmetry of S_{ij} can be maintained by writing [3]:

$$S_{ij} = \frac{1}{2}\left(\frac{\partial W}{\partial E_{ij}} + \frac{\partial W}{\partial E_{ji}}\right) \tag{1.6}$$

Assuming that $a_1 = 2\ a_2 = a_3 = a$ [2] and using equation 1.6 we obtain: (appendix A)

$$\mathcal{S} = 2\,a\,W(\mathcal{E}) \begin{bmatrix} E_{11} & E_{12} & E_{13} \\ E_{21} & E_{22} & E_{23} \\ E_{31} & E_{32} & 2E_{33} \end{bmatrix} + a_4\,W(\mathcal{E}) \begin{bmatrix} 0 & 0 & E_{13} \\ 0 & 0 & E_{23} \\ E_{31} & E_{32} & 0 \end{bmatrix} \tag{1.7}$$

1.2.3 Strain-energy function by Huyghe

To describe the passive behaviour of myocardial tissue (orthotropic), Huyghe [4] specified the strain-energy function W by:

$$\begin{aligned} W(\mathcal{E}) = \;& c_n \;\; \{exp\,(a_{cf}E_{11}) - a_{cf}E_{11} + exp\,(a_{cf}E_{22}) - a_{cf}E_{22} + exp\,(a_fE_{33}) - a_fE_{33} \\ & + \;[exp\,(a_bE_{11}) - a_bE_{11}]\,[exp\,(a_bE_{22}) - a_bE_{22}] \\ & + \;[exp\,(a_bE_{11}) - a_bE_{11}]\,[exp\,(a_bE_{33}) - a_bE_{33}] \\ & + \;[exp\,(a_bE_{22}) - a_bE_{22}]\,[exp\,(a_bE_{33}) - a_bE_{33}] \;- 6\} \\ & + \;c_s\{exp\,[a_s(E_{12}E_{12} + E_{13}E_{13} + E_{23}E_{23})] - 1\} \end{aligned} \tag{1.8}$$

where:

c_n = initial normal stiffness
c_s = initial shear stiffness
a_{cf} = exponential factor in cross-fiber stiffness
a_f = exponential factor in fiber stiffness
a_b = exponential factor in bi-axial stiffness
a_s = exponential factor in shear stiffness

The above strain-energy function assumes implicitely that the stress-strain relationships in direction 1 (transmural) and direction 2 (plane cross-fiber direction) are the same.

Using equation 1.6 we obtain: (appendix A)

$$\begin{aligned} S_{ii} &= c_n\{a_{cf}E_{ii} - a_{cf} + a_b\,exp\,(a_bE_{ii} + E_{jj}) - a_b exp\,(a_bE_{jj}) \quad && i=1 \quad j=2,3 \\ &\quad -{a_b}^2E_{jj}exp\,(a_bE_{ii}) + {a_b}^2E_{jj}\} && i=2 \quad j=1,3 \\ & && i=3 \quad j=1,2 \\ S_{ij} &= \tfrac{1}{2}c_s\{2a_sE_{ij}exp\,(a_s(E_{12}E_{12} + E_{13}E_{13} + E_{23}E_{23}))\} && i,j = 1,2,3 \\ & && i \neq j \end{aligned} \tag{1.9}$$

1.3 Simple test problems

Our aim is to implement the non-linear elastic constitutive equations in the Finite Element Package DIANA [5]. If we want to test these implemented equations it is necessary to compare the output of DIANA with analytical solutions. Therefore the analytical solutions for two different (simple) test problems are derived: uniaxial stretch and simple shear.

1.3.1 Uniaxial stretch and compression

Consider a uniform compression or extension of the block in figure 1.1, in the $\vec{e}_3$-direction. It's length changes from l_{30} to l_3, and its cross-section changes from A_0 to A.

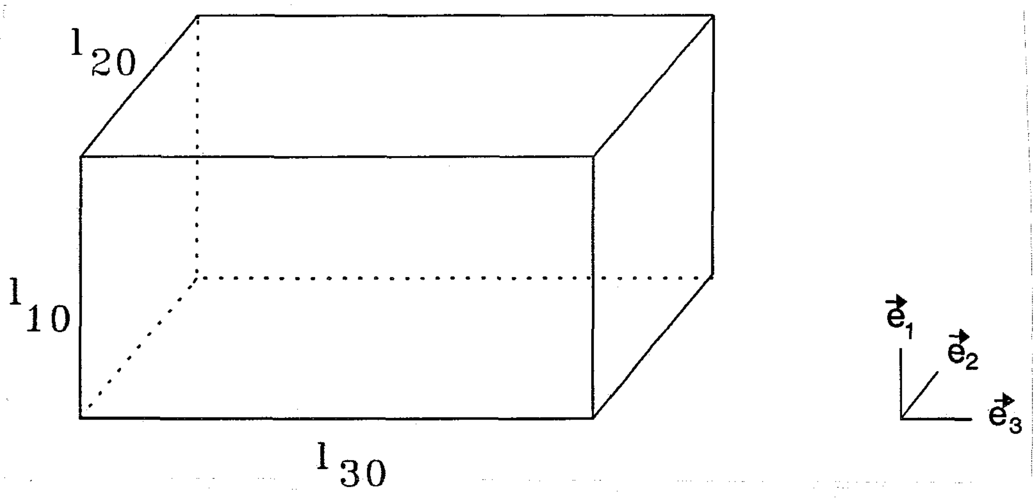

Figure 1.1: deformation of a block

The deformation gradient tensor $\mathcal{F}$ depends on the material symmetry:

* isotropic/ transversely isotropic $\vec{e}_3$-direction

$$\mathcal{F} = \begin{pmatrix} \lambda_2 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_1 \end{pmatrix} \qquad \lambda_1 = \frac{l_3}{l_{30}} \qquad \lambda_2 = \sqrt{\frac{A}{A_0}} \tag{1.10}$$

* orthotropic

$$\mathcal{F} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \qquad \lambda_1 = \frac{l_1}{l_{10}} \qquad \lambda_2 = \frac{l_2}{l_{20}} \qquad \lambda_3 = \frac{l_3}{l_{30}} \tag{1.11}$$

1. Uniaxial stretch/compression in the model of Mow/Holmes

The equation for the 2nd Piola-Kirchhoff tensor has been derived in section 1.2.1 (equation 1.4).

$$\mathcal{P} = 2\,W\,\{(\alpha_1 + \alpha_2 J_1 - \frac{J2}{J3}\,\beta)\mathcal{I} + (-\alpha_2 + \frac{J_1}{J_3}\,\beta)\mathcal{C} - \frac{\beta}{J_3}\,\mathcal{C}^2\}$$

The Cauchy-Green strain tensor $\mathcal{C}$ for isotropic uniaxial stretch/compression yields:

$$\mathcal{C} = \mathcal{F}^c.\mathcal{F} = \begin{pmatrix} \lambda_2^2 & 0 & 0 \\ 0 & \lambda_2^2 & 0 \\ 0 & 0 & \lambda_1^2 \end{pmatrix} \tag{1.12}$$

where:
$J_1 = tr(\mathcal{C}) = \lambda_1^2 + 2\,\lambda_2^2$
$J_2 = \frac{1}{2}\,\{\,(tr\,(\mathcal{C})^2)\text{-}\,tr(\mathcal{C}^2)\,\} = 2\,\lambda_1^2\lambda_2^2 + \lambda_2^4$
$J_3 = det(\,\mathcal{C}\,) = \lambda_1^2\lambda_2^4$

substitution of this equation in equation 1.4 gives:

$$\begin{aligned} P_{11} &= 2\rho_0 W[\alpha_1 + \alpha_2\lambda_1^2 + \alpha_2\lambda_2^2 - \frac{\beta}{\lambda_2^2}] \\ P_{22} &= 2\rho_0 W[\alpha_1 + \alpha_2\lambda_1^2 + \alpha_2\lambda_2^2 - \frac{\beta}{\lambda_2^2}] \\ P_{33} &= 2\rho_0 W[\alpha_1 + 2\alpha_2\lambda_2^2 - \frac{\beta}{\lambda_1^2}] \end{aligned} \tag{1.13}$$

where:

$$W = \alpha_0 \frac{exp\,(\alpha_1(\lambda_1^2 + 2\lambda_2^2 - 3) + \alpha_2(2\lambda_1^2\lambda_2^2 + \lambda_2^4 - 3))}{(\lambda_1^2\lambda_2^4)^\beta} \tag{1.14}$$

It is difficult to interpret the second Piola-Kirchoff stress tensor. Therefore the first Piola-Kirchhoff stress tensor ($\mathcal{T}$) is used. $\mathcal{T}$ is directly related to the force on an undeformed surface.

$$\mathcal{T} = \mathcal{P}.\mathcal{F}^c \tag{1.15}$$

In this case:

$$\mathcal{T} = \begin{pmatrix} \lambda_2 P_{11} & 0 & 0 \\ 0 & \lambda_2 P_{22} & 0 \\ 0 & 0 & \lambda_1 P_{33} \end{pmatrix} \tag{1.16}$$

In the case of uni-axial stretch/compression in $\vec{e}_3$-direction, T_{11} and T_{22} have to be zero.

$$T_{11} = T_{22} = \lambda_2[2\rho_0 W(\alpha_1 + \alpha_2\lambda_1^2 + \alpha_2\lambda_2^2 - \frac{\beta}{\lambda_2^2})] = 0 \tag{1.17}$$

The relevant solution of this equation yields:

$$\lambda_2^2 = \frac{-\alpha_1 - \alpha_2\lambda_1^2 + \sqrt{(\alpha_1 + \alpha_2\lambda_1^2)^2 + 4\alpha_2\beta}}{2\alpha_2} \tag{1.18}$$

Substituting λ_2^2 in T_{33} gives:

$$T_{33} = \lambda_1 P_{33} = \lambda_1\, W\,[-\alpha_2\lambda_1^2 + \sqrt{(\alpha_1 + \alpha_2\lambda_1^2)^2 + 4\alpha_2\beta} - \frac{\beta}{\lambda_1^2}] \tag{1.19}$$

In the next figure T33 is given as a function of λ_1:

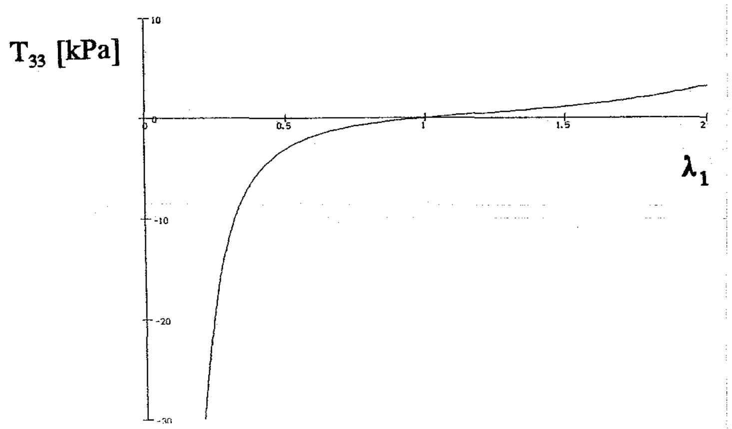

Figure 1.2: T 33 as a function of λ_1, where α_0=1, α_1=0.3 and α_2=0.2.

2. uni-axial stretch/compression in the model of Bovendeerd

The equation for the 2nd Piola-Kirchhoff stress tensor has been derived in section 1.2.2:

$$\mathcal{S} = 2\,a\,W(\mathcal{E}) \begin{bmatrix} E_{11} & E_{12} & E_{13} \\ E_{21} & E_{22} & E_{23} \\ E_{31} & E_{32} & 2E_{33} \end{bmatrix} + a_4\,W(\mathcal{E}) \begin{bmatrix} 0 & 0 & E_{13} \\ 0 & 0 & E_{23} \\ E_{31} & E_{32} & 0 \end{bmatrix}$$

The Green-Lagrange strain tensor $\mathcal{E}$ for transversely isotropic uni-axial stretch/compression yields:

$$\mathcal{E} = \frac{1}{2}(\mathcal{F}.\mathcal{F}^c - \mathcal{I}) = \frac{1}{2}\begin{pmatrix} \lambda_2^2 - 1 & 0 & 0 \\ 0 & \lambda_2^2 - 1 & 0 \\ 0 & 0 & \lambda_1^2 - 1 \end{pmatrix} \tag{1.20}$$

Substituting equation 1.20 in equation 1.7:

$$\begin{aligned} S_{11} &= a\, W(\mathcal{E})(\lambda_2^2 - 1) \\ S_{22} &= a\, W(\mathcal{E})(\lambda_2^2 - 1) \\ S_{33} &= a\, W(\mathcal{E})(\lambda_1^2 - 1) \end{aligned} \tag{1.21}$$

where:

$$W(\mathcal{E}) = c[exp\,(\frac{1}{4}a(\lambda_1^2 - 1)^2) - 1] \tag{1.22}$$

In this case T_{11} and T_{22} have to be zero.

$$T_{11} = T_{22} = \lambda_2 S_{11} = \lambda_2\, a\, W(\mathcal{E})\,(\lambda_2^2 - 1) = 0 \tag{1.23}$$

The only solution for this equation is $\lambda_2 = 1$.

$$T_{33} = \lambda_2 S_{33} = a\, W(\mathcal{E})\,(\lambda_1^2 - 1) \tag{1.24}$$

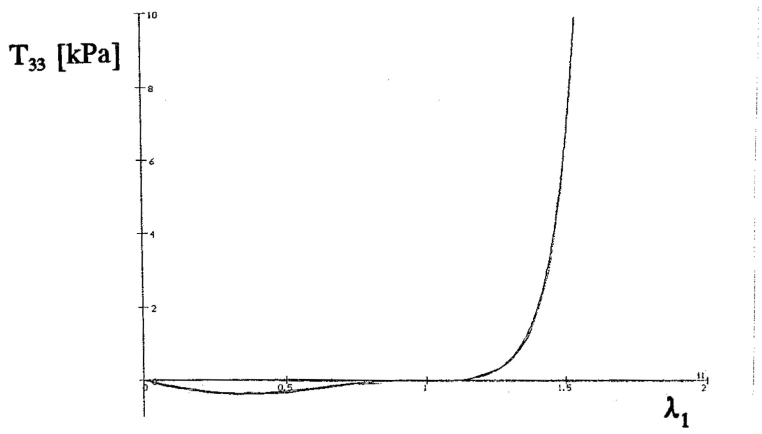

Figure 1.3: T_{33} as a function of λ_1, a=3 and c=0.5 [kPa]

3. Uniaxial stretch/compression in the model of Huyghe

In section 1.2.3 the 2nd Piola-Kirchhoff stress tensor for the model of Huyghe has been derived.

$$\begin{aligned} S_{ii} &= c_n\{a_{cf}E_{ii} - a_cf + a_b\, exp\,(a_bE_{ii} + E_{jj}) - a_b exp\,(a_bE_{jj}) && i=1 \quad j=2,3 \\ &\quad -a_b{}^2E_{jj}exp\,(a_bE_{ii}) + a_b{}^2E_{jj}\} && i=2 \quad j=1,3 \\ & && i=3 \quad j=1,2 \qquad (1.25) \\ S_{ij} &= \tfrac{1}{2}c_s\{2a_sE_{ij}exp\,(a_s(E_{12}E_{12}+E_{13}E_{13}+E_{23}E_{23}))\} && i,j = 1,2,3 \\ & && i\neq j \end{aligned}$$

For orthotropic uni-axial stretch/compression the Green-Lagrange strain tensor yields:

$$\mathcal{E} = \frac{1}{2}\begin{pmatrix} \lambda_1^2-1 & 0 & 0 \\ 0 & \lambda_2^2-1 & 0 \\ 0 & 0 & \lambda_3^2-1 \end{pmatrix} \tag{1.26}$$

Combining these equations and equation 1.15 gives:

$$\begin{aligned} T_{11} = \ & \lambda_1 \quad c_n\{a_{cf}exp\,(a_{cf}\frac{1}{2}(\lambda_1^2-1)) - a_{cf} + a_b exp\,(a_b\frac{1}{2}(\lambda_1^2-1) + a_b\frac{1}{2}(\lambda_2^2-1)) \\ - & \quad a_b exp\,\frac{1}{2}(a_b(\lambda_2^2-1) - a_b^2\frac{1}{2}(\lambda_2^2-1)exp\,(a_b\frac{1}{2}(\lambda_1^2-1)) + a_b^2\frac{1}{2}(\lambda_2^2-1) \\ + & \quad a_b exp\,(a_b\frac{1}{2}(\lambda_1^2-1) + a_b\frac{1}{2}(\lambda_3^2-1)) - a_b^2\frac{1}{2}(\lambda_3^2-1)exp\,(a_b\frac{1}{2}(\lambda_1^2-1)) \\ - & \quad a_b exp\,(a_b\frac{1}{2}(\lambda_3^2-1)) + a_b^2\frac{1}{2}(\lambda_3^2-1)\} \end{aligned} \tag{1.27}$$

$$\begin{aligned} T_{22} = \ & \lambda_2 \quad c_n\{a_{cf}exp\,(a_{cf}\frac{1}{2}(\lambda_2^2-1) - a_{cf} + a_b exp\,(a_b\frac{1}{2}(\lambda_1^2-1) + a_b\frac{1}{2}(\lambda_2^2-1)) \\ - & \quad a_b^2\frac{1}{2}(\lambda_1^2-1)exp\,(a_b\frac{1}{2}(\lambda_2^2-1)) - a_b exp\,(a_b\frac{1}{2}(\lambda_1^2-1) + a_b^2\frac{1}{2}(\lambda_1^2-1) \\ + & \quad a_b exp\,(a_b\frac{1}{2}(\lambda_2^2-1) + a_b\frac{1}{2}(\lambda_3^2-1)) - a_b^2\frac{1}{2}(\lambda_3^2-1)exp\,(a_b\frac{1}{2}(\lambda_2^2-1)) \\ - & \quad a_b exp\,(a_b\frac{1}{2}(\lambda_3^2-1)) + a_b^2\frac{1}{2}(\lambda_3^2-1)\} \end{aligned} \tag{1.28}$$

$$\begin{aligned} T_{33} = \ & \lambda_3 \quad c_n\{a_{cf}exp\,(a_{cf}\frac{1}{2}(\lambda_3^2-1) - a_{cf} + a_b exp\,(a_b\frac{1}{2}(\lambda_1^2-1) + a_b\frac{1}{2}(\lambda_3^2-1)) \\ - & \quad a_b exp\,(a_b\frac{1}{2}(\lambda_1^2-1) - a_b^2\frac{1}{2}(\lambda_1^2-1)exp\,(a_b\frac{1}{2}(\lambda_3^2-1)) + a_b^2\frac{1}{2}(\lambda_1^2-1) \\ + & \quad a_b exp\,(a_b\frac{1}{2}(\lambda_2^2-1) + a_b\frac{1}{2}(\lambda_3^2-1)) - a_b exp\,(a_b\frac{1}{2}(\lambda_2^2-1)) \\ - & \quad a_b^2\frac{1}{2}(\lambda_2^2-1)exp\,(a_b\frac{1}{2}(\lambda_3^2-1)) + a_b^2\frac{1}{2}(\lambda_2^2-1)\} \end{aligned} \tag{1.29}$$

In the case of uni-axial stretch T_{11} and T_{22} have to be zero.

$$T_{11} = 0 \qquad \lambda_1^2 = 1$$
$$T_{22} = 0 \qquad \lambda_2^2 = 1$$

Substituting λ_1^2 and λ_2^2 in T_{33} yields:

$$T_{33} = \lambda_3 c_n \{a_{cf} exp\,(\frac{1}{4} a_{cf}(\lambda_3^2 - 1)) - a_{cf} + 2a_b exp\,(\frac{1}{4} a_b(\lambda_3^2 - 1)) - 2a_b\} \tag{1.30}$$

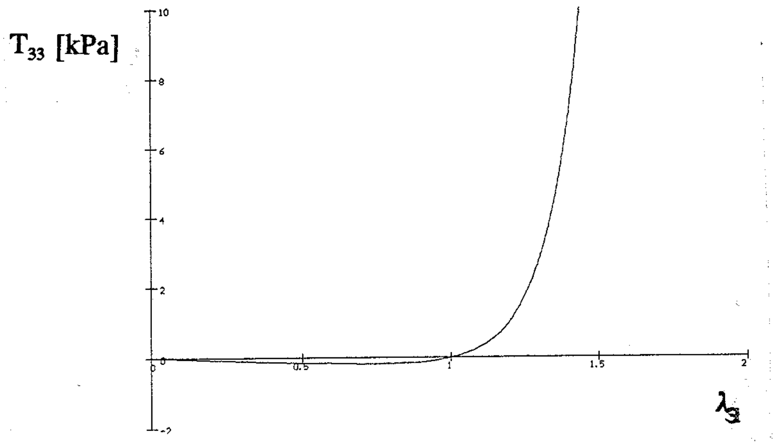

Figure 1.4: T_{33} as a function of λ_3 where c_n=0.01 [kPa], a_{cf}=10, a_b=12.

1.3.2 Simple shear

The top surface of the block in figure 1.1 is subjected to a translation in the $\vec{e}_3$-direction (u_3), while the bottom surface is fixed. The deformation gradient matrix F for this proces is:

* isotropic/ transversely isotropic/ orthotropic

$$F = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \gamma & 0 & 1 \end{pmatrix} \qquad \gamma = \left[\frac{u_3}{l_{10}}\right] \tag{1.31}$$

1. Simple shear in the model of Mow/Holmes

In the case of simple shear the Cauchy-Green strain tensor yields:

$$\mathcal{C} = \mathcal{F}^c \mathcal{F} = \begin{pmatrix} 1+\gamma^2 & 0 & \gamma \\ 0 & 1 & 0 \\ \gamma & 0 & 1 \end{pmatrix} \tag{1.32}$$

Using equation 1.4, 1.15 and 1.32 we obtain:

$$\begin{aligned} T_{11} &= 0 \\ T_{22} &= 2\rho_0\, W\,(\alpha_2\,\gamma^2) \\ T_{33} &= 0 \\ T_{13} &= T_{31} = 2\,\rho_0\, W\,\{(-\alpha_2+\beta)\,\gamma\} \end{aligned} \tag{1.33}$$

where:

$$W = \frac{\alpha_0}{\rho_0}\, exp\,((\alpha_1+\alpha_2)\gamma^2) \tag{1.34}$$

These functions are shown in the next figure:

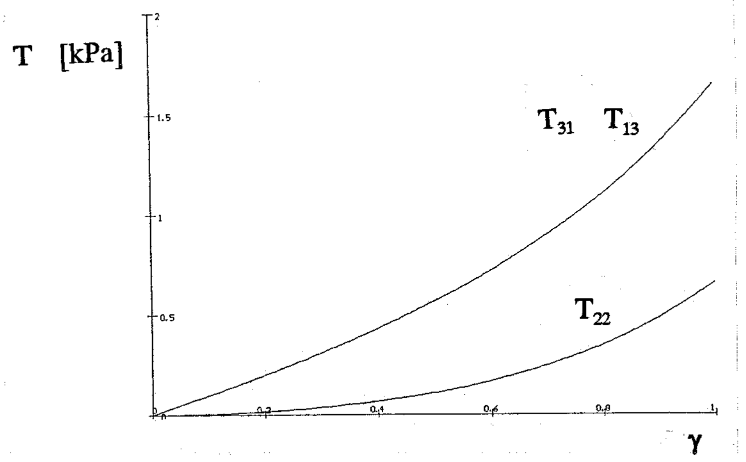

Figure 1.5: T_{22}, T_{13} and T_{31} as a function of γ where α_0=1 , α_1=0.3 and α_2=0.2.

2. Simple shear in the model of Bovendeerd

In the case of simple shear the Green-Lagrange strain tensor yields:

$$\mathcal{E} = \frac{1}{2}(\mathcal{F}^c.\mathcal{F}-\mathcal{I}) = \frac{1}{2}\begin{pmatrix} \gamma^2 & 0 & \gamma \\ 0 & 0 & 0 \\ \gamma & 0 & 0 \end{pmatrix} \tag{1.35}$$

Using equation 1.7, 1.15 and 1.35:

$$\begin{aligned} T_{11} &= a\,W(\mathcal{E})\,\gamma^2 \\ T_{22} &= 0 \\ T_{33} &= \gamma^2(a\,W(\mathcal{E}) + \tfrac{1}{2}a_4\,W(\mathcal{E})) \\ T_{13} &= \gamma(a\,W(\mathcal{E}) + \gamma^2\,a\,W(\mathcal{E}) + \tfrac{1}{2}a_4 W(\mathcal{E})) \\ T_{31} &= \gamma(a\,E(\mathcal{E}) + \tfrac{1}{2}a_4 W(\mathcal{E})) \end{aligned} \tag{1.36}$$

where:

$$W(\mathcal{E}) = c[exp\,(\frac{1}{4}\gamma^2(a\gamma^2 + 2a + a_4)) - 1] \tag{1.37}$$

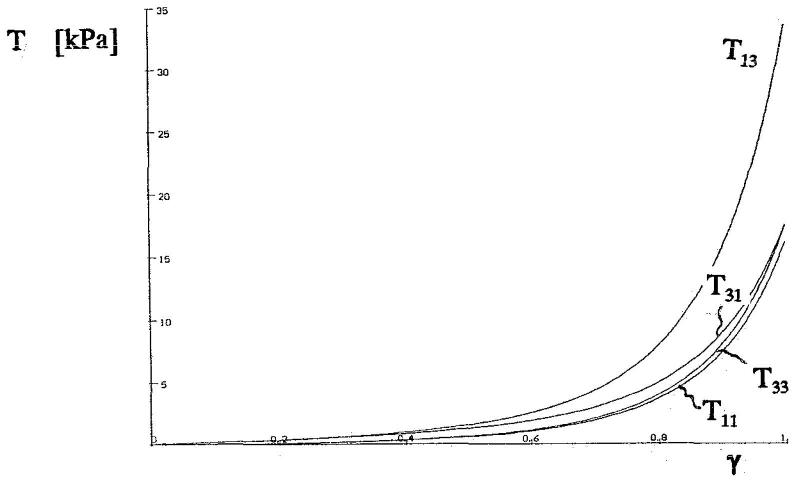

Figure 1.6: T_{11}, T_{33}, T_{13} and T_{31} as a function of γ where a=3, c=0.5 [kPa] and a_4=0.5.

3. Simple shear in the model of Huyghe

Using equation 1.9 , 1.15 and 1.35 it is possible to derive:

$$\begin{aligned}
T_{11} &= c_n\{a_{cf}exp\,(\tfrac{1}{2}a_{cf}\gamma^2) - a_{cf} + 2a_b exp\,(\tfrac{1}{2}a_b\gamma^2) - 2a_b\}\\
T_{22} &= 0\\
T_{33} &= \tfrac{1}{2}c_s a_s\gamma^2 exp\,(\tfrac{1}{4}\gamma^2)\\
T_{13} &= \tfrac{1}{2}c_s a_s\gamma^2 exp\,(\tfrac{1}{4}\gamma^2) + \gamma c_n\{a_{cf}exp\,(\tfrac{1}{2}a_{cf}\gamma^2) - a_{cf} + 2a_b exp\,(\tfrac{1}{2}a_b\gamma^2) - 2a_b\}\\
T_{31} &= \tfrac{1}{2}c_s a_s\gamma exp\,(\tfrac{1}{4}\gamma^2)
\end{aligned} \tag{1.38}$$

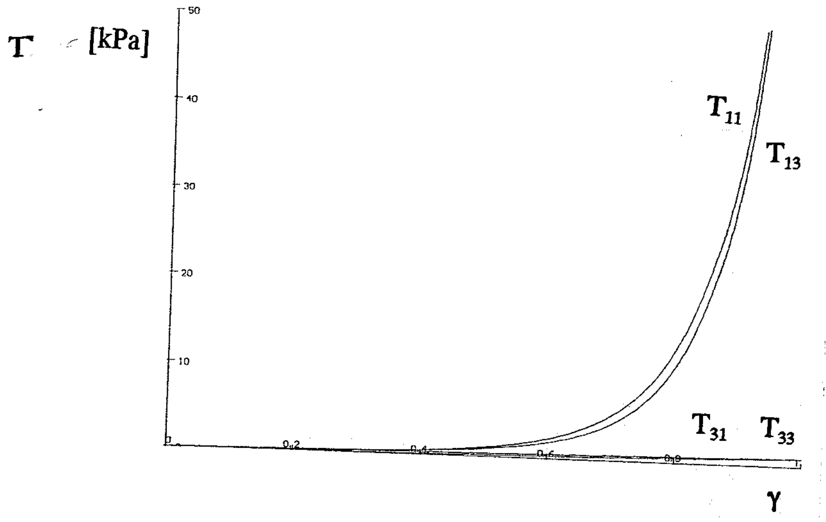

Figure 1.7: T_{11}, T_{33}, T_{13} and T_{31} as a function of γ where c_n=0.01 [kPa], a_{cf}=10, a_b=12, c_s=0.1 [kPa] and a_s=15.

1.3.3 Summary

		Holmes/Mow	Bovendeerd	Huyghe
Uni- axial tensile test	T_{33}	$\lambda_1 2\rho_0 W[\alpha_1 + 2\alpha_2\lambda_2^2 - \frac{b}{\lambda_1^2}]$ where: $\lambda_2^2 = \frac{-\alpha_1 - \alpha_2\lambda_2^2 + \sqrt{(\alpha_1+\alpha_2\lambda_1^2)^2 + 4\alpha_2\beta}}{2\alpha_2}$ $W = \frac{\alpha_0}{\rho_0}\frac{exp\,(\alpha_1(\lambda_1^2+2\lambda_2^2-3)+\alpha_2(2\lambda_1^2\lambda_2^2+\lambda_2^4-3))}{(\lambda_1^2\lambda_2^4)^\beta}$ b=$\alpha_1 + 2\alpha_2$	$\lambda_1 a W(\lambda_1^2 - 1)$ where: $W = c[exp\,(\frac{1}{4}a(\lambda_1^2-1)^2) - 1]$ N.B. $\lambda_2 = 1$	$\lambda_3 c_n\{a_{cf} exp\,(\frac{1}{2}a_{cf}(\lambda_3^2 - 1))$ $-a_{cf} + 2a_b exp\,(\frac{1}{2}a_b(\lambda_3^2-1)) - 2a_b\}$ N.B. $\lambda_1^2 = 1$ $\lambda 2^2 = 1$
Simple	T_{11}	0	a W γ^2	$c_n[a_{cf} exp\,(\frac{1}{2}a_{cf}\gamma^2) - a_{cf}] +$ $2a_b exp\,(\frac{1}{2}a_b\gamma^2) - 2a_b$
shear	T_{22}	$2\rho_0 W(\alpha_2\gamma^2)$	0	0
	T_{33}	0	$\gamma^2 W(a + \frac{1}{2}a_4)$	$\frac{1}{2}c_s a_s \gamma^2 exp\,(\frac{1}{4}\gamma^2)$
	T_{13}	$2\rho_0 W[(\alpha_1+\alpha_2)\gamma]$	$\gamma W(a + a\gamma^2 + \frac{1}{2}a_4)$	$\frac{1}{2}c_s a_s \gamma^2 exp\,(\frac{1}{4}\gamma^2) + \gamma c_n[a_{cf} exp\,(\frac{1}{2}a_{cf}\gamma^2)$ $-a_{cf} + 2a_b exp\,(\frac{1}{2}a_b\gamma^2) - 2a_b]$
	T_{31}	$2\rho_0 W[(\alpha_1+\alpha_2)\gamma]$	$\gamma W(a + \frac{1}{2}a_4)$	$\frac{1}{2}c_s a_s \gamma exp\,(\frac{1}{4}\gamma^2)$
		where: $W = \frac{\alpha_0}{\rho_0} exp\,(\gamma^2(\alpha_1+\alpha_2))$	where: $W = c[exp\,\frac{1}{4}\gamma^2(a\gamma^2 + 2a + a_4) - 1]$	

In uniaxial compression the models of Bovendeerd and Huyghe predict $T_{11} = 0$ for λ_1 (λ_3) = 0. In practice T_{11} has to go to minus infinity as λ_1 (λ_3) approaches zero.

It is also remarkable that in the simple shear situation the model of Mow/Holmes (T_{11}, $T_{33} = 0$; $T_{22} \neq 0$) predicts the opposite of the models of Bovendeerd and Huyghe (T_{11}, $T_{33} \neq 0$; $T_{22} = 0$). In the simple shear situation, T_{11} can't be zero. This can be made clearly from the following figure:

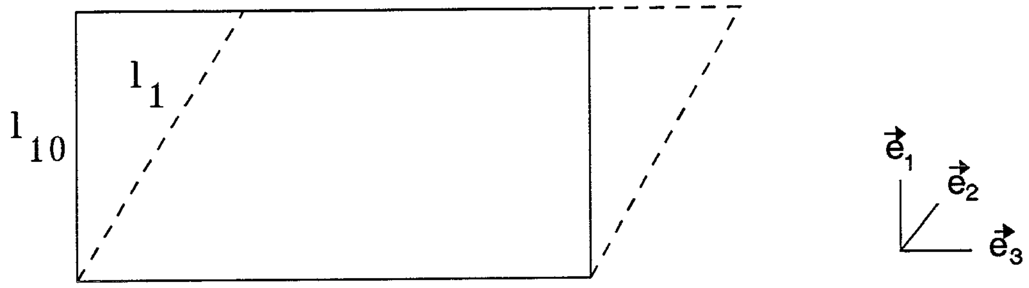

Figure 1.8: deformation block in simple shear

The upper plane moves to the right, but stays at the same height $l_1 > l_{10}$. To achieve this there must be a force on the block in 11-direction. The model of Mow/Holmes must therefore be distrusted in shear stuations.

1.4 Plane stress situation

We want to use a membrane element in DIANA. The behaviour of this element can be described in a plane stress situation. To compare the DIANA-results for this element with analytical results, the equations of the 2nd Piola-Kirchhoff stress tensor have to be rewritten to the plane-stress situation. In the next subsections this will be done for the models of Mow/Holmes, Bovendeerd and Huyghe.

In the plane-stress situation it is assumed that the 13-, 23- and 33-components of the stress tensor are zero. With the equation $P(S)_{33} = 0$, it is sometimes possible to express $E_{33}(C_{33})$ as a function of $E_{11}(C_{11})$ and $E_{22}(C_{22})$. Substituting the equation for C_{33} in S_{11} and S_{22} yields the 2nd Piola-Kirchhoff stress tensor for the plane- stress situation.

If it is not possible to express E_{33} as a function of E_{11} and E_{22}, E_{33} is left out of the strain-energy function. Because $S_{33} = \frac{\partial W(E)}{\partial E_{33}}$, leaving E_{33} out ensures that $S_{33} = 0$. From the new strain-energy function the 2nd Piola- Kirchhoff stress tensor for plane stress can be derived. In the first situation the coefficients of plane-stress can be used in the 3-D situation. In the second situation this is not possible.

1.4.1 Plane stress in the model of Mow/Holmes

The 2nd Piola-Kirchhoff stress tensor in the model of Mow/Holmes yields:

$$\mathcal{P} = 2\rho_0\, W\,\{(\alpha_1 + \alpha_2 J_1 - \frac{J_2}{J_3}\,\beta)\,\mathcal{I} + (-\alpha_2 + \frac{J_1}{J_3}\,\beta)\mathcal{C} - \frac{\beta}{J_3}\,\mathcal{C}^2\} \tag{1.39}$$

In the case of plane stress, C_{13}, C_{23}, P_{13}, P_{23} and P_{33} are zero.

$$P_{33} = 2\rho_0 W(\alpha_1 + \alpha_2 J_1 - \frac{J_2}{J_3}\beta) + (-\alpha_2 + \frac{J_1}{J_3}\beta)C_{33} - \frac{\beta}{J_3}C_{33}^2 = 0 \tag{1.40}$$

where:
$J_1 = C_{11} + C_{22} + C_{33}$
$J_2 = C_{11}C_{22} + C_{22}C_{33} + C_{11}C_{33} - C_{12}^2$
$J_3 = C_{11}C_{22}C_{33} - C_{12}^2\, C_{33}$
$\beta = \alpha_1 + 2\,\alpha_2$
$W(E) = \frac{\alpha_0}{\rho_0}\frac{exp\,(\alpha_1(J_1-3)+\alpha_2(J_2-3))}{J_3{}^{\beta}}$

It is now possible to express C_{33} as a function of C_{11} and C_{22}:

$$C_{33} = \frac{\beta}{\alpha_2 C_{11} + \alpha_2 C_{22} + \alpha_1} \tag{1.41}$$

Substituting C_{33} in equation 1.4, we obtain the 2nd Piola-Kirchhoff stress P_{11}, P_{22} and P_{12}, for plane stress:

$$\begin{aligned} P_{11} &= 2\rho_0 W(\alpha_1 + \alpha_2 J_1 - \frac{J_2}{J_3}\beta) + (-\alpha_2 + \frac{J_1}{J_3}\beta)\, C_{11} - \frac{\beta}{J_3}(C_{11}^2 + C_{12}^2) \\ P_{22} &= 2\rho_0 W(\alpha_1 + \alpha_2 J_1 - \frac{J_2}{J_3}\beta) + (-\alpha_2 + \frac{J_1}{J_3}\beta)\, C_{22} - \frac{\beta}{J_3}(C_{12}^2 + C_{22}^2) \\ P_{12} &= 2\rho_0 W(-\alpha_2 + \frac{J_1}{J_3}\beta)\, C_{12} - \frac{\beta}{J_3}(C_{11}C_{12} + C_{22}C_{12}) \end{aligned} \tag{1.42}$$

1.4.2 Plane stress in the model of Bovendeerd

In plane stress the equation for S_{33} in this model yields: (E_{13}, $E_{23} = 0$)

$$S_{33} = 4aW(E)E_{33} = 0 \tag{1.43}$$

The only solution is E_{33}=0. This means that in this model plane stress and plane strain are the same. In practice this is not very plausible. With S_{33}, E_{13},E_{23} and E_{33} we obtain:

$$\mathcal{S} = 2aW(E)\begin{pmatrix} E_{11} & E_{12} \\ E_{12} & E_{22} \end{pmatrix} \tag{1.44}$$

Because we left out the $\vec{e}_3$-direction in this 2nd Piola-Kirchhoff stress tensor, this equation is now isotropic. ($\vec{e}_1$,$\vec{e}_2$-plane was isotropic)

1.4.3 Plane stress in the model of Huyghe

The equation for S_{33} yields:

$$\begin{aligned} S_{33} = \left(\frac{\partial W}{\partial E_{33}}\right) &= c_n\{a_{cf}exp\,(a_{cf}E_{33}) - a_{cf} + a_b exp\,(a_b E_{11} + a_b E_{33}) - a_b exp\,(a_b E_{11}) \\ &- a_b^2 E_{11} exp\,(a_b E_{33}) + a_b^2 E_{11} + a_b exp\,(a_b E_{22} + a_b E_{33}) \\ &- a_b exp\,(a_b E_{22}) - a_b^2 E_{22} exp\,(a_b E_{33}) + a_b^2 E_{22}\} \end{aligned} \tag{1.45}$$

This equation can be rewritten to the basic form:

$$S_{33} = ay^b + cy^d + e = 0 \tag{1.46}$$

Solving this equation means that $ay^b + cy^d = e$, where b and d are unknown. This can only be done numerically. Therefore the second method is used. Leaving E_{33}, E_{13} and E_{23} out of the strain-energy function gives:

$$\begin{aligned} W(E) = \; & c_n \quad \{exp\,(a_{cf}E_{11}) - a_{cf}E_{11} + exp\,(a_{cf}E_{22}) - a_{cf}E_{22} \\ + \; & [exp\,(a_bE_{11}) + a_bE_{11}][exp\,(a_bE_{22}) + a_bE_{22}]\} \\ + \; & c_s\{exp\,(asE_{12}E_{12})\} \end{aligned} \tag{1.47}$$

The elements of the 2nd Piola-Kirchhoff stress tensor for plane stress are:

$$\begin{aligned} S_{11} = \frac{\partial W}{\partial E_{11}} = \; & c_n \quad \{a_{cf}exp\,(a_{cf}E_{11}) - a_{cf} + a_bexp\,(a_bE_{11} + a_bE_{22}) \\ - \; & a_b^2E_{22}exp\,(a_bE_{11}) - a_bexp\,(a_bE_{22}) + a_b^2E_{22}\} \end{aligned} \tag{1.48}$$

$$\begin{aligned} S_{22} = \frac{\partial W}{\partial E_{22}} = \; & c_n \quad \{a_{cf}exp\,(a_{cf}E_{22}) - a_{cf} + a_bexp\,(a_bE_{11} + a_bE_{22}) \\ - \; & a_bexp\,(a_bE_{11}) - a_b^2E_{11}exp\,(a_bE_{22}) + a_b^2E_{11}\} \end{aligned} \tag{1.49}$$

$$S_{12} = S_{21} = \frac{1}{2}\left(\frac{\partial W}{\partial E_{12}} + \frac{\partial W}{\partial E_{21}}\right) = c_sa_sE_{12}exp\,(a_sE_{12}E_{12}) \tag{1.50}$$

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Appendix A

In this appendix the derivation of the 2nd Piola-Kirchhoff stress tensor for three different strain-energy functions will be made.

A.1 Mow/Holmes

Mow and Holmes use the following strain-energy function:

$$\rho_0\psi(\mathcal{C}) = W(\mathcal{C}) = \alpha_0 \, \frac{exp\,(\alpha_1\,(J_1 - 3) + \alpha_2\,(J_2 - 3))}{{J_3}^{\beta}} \tag{A.1}$$

where:
ψ = free energy
ρ_0 = mass density
$\alpha_0, \alpha_1, \alpha_2$= positive constants
$\beta = \alpha_1 + 2\alpha_2$
J_1, J_2, J_3 = three principal invariants of the Cauchy Green strain tensor

The 2nd Piola-Kirchhoff stress tensor can be related to the strain-energy function:

$$\begin{aligned} \mathcal{P} &= 2\,\frac{\partial W(\mathcal{C})}{\partial \mathcal{C}} \\ &= 2\,\left(\frac{\partial W}{\partial (J_1)}\,\frac{\partial (J_1)}{\partial \mathcal{C}} + \frac{\partial W}{\partial (J_2)}\,\frac{\partial (J_2)}{\partial \mathcal{C}} + \frac{\partial W}{\partial (J_3)}\,\frac{\partial (J_3)}{\partial \mathcal{C}}\right) \end{aligned} \tag{A.2}$$

The derivates of the invariants to the Cauchy-Green strain tensor have the following form:

$$\frac{\partial (J_1)}{\partial \mathcal{C}} = \mathcal{I} \qquad \frac{\partial (J_2)}{\partial \mathcal{C}} = J_1\,\mathcal{I} - \mathcal{C} \qquad \frac{\partial (J_3)}{\partial \mathcal{C}} = J_2\,\mathcal{I} - J_1\mathcal{C} + \mathcal{C}^2 \tag{A.3}$$

It is now possible to determine the 2nd Piola-Kirchhoff stress for the model of Mow and Holmes:

$$\begin{aligned}\mathcal{P} = 2\{ \quad & \alpha_0 \quad \frac{exp\,(\alpha_1(J_1-3)+\alpha_2(J_2-3))}{J_3{}^{\beta}}\,\alpha_1 \mathcal{I} \, + \\ & \alpha_0 \quad \frac{exp\,(\alpha_1(J_1-3)+\alpha_2(J_2-3))}{J_3{}^{\beta}}\,\alpha_2\,(\,J_1\mathcal{I}-\mathcal{C})\, + \\ & \alpha_0 \quad \frac{exp\,(\alpha_1(J_1-3)+\alpha_2(J_2-3))\;*(-\beta)}{J_3{}^{\beta+1}}\,(J_2\,\mathcal{I}-J_1\,\mathcal{C}+\mathcal{C}^2)\}\end{aligned}$$

$$\mathcal{P} = 2\,W\,\{(\alpha_1+\alpha_2 J_1 - \frac{J_2}{J_3}\beta)\,\mathcal{I} \; + \; (-\alpha_2 + \frac{J_1}{J_3}\beta)\mathcal{C} \; - \; \frac{\beta}{J_3}\,\mathcal{C}^2\} \tag{A.4}$$

A.2 Bovendeerd

Bovendeerd uses the strain-energy function:

$$W(\mathcal{E}) = c\,[exp\,(a_1\,I_E{}^2 + a_2\,II_E + a_3\,I_E'^{\,2} + a_4\,II_E'^{\,2}) - 1] \tag{A.5}$$

where:
$I_E = E_{11} + E_{22} + E_{33}$
$II_E = E_{12}^2 + E_{23}^2 + E_{31}^2 - E_{11}\,E_{22} - E_{22}E_{33} - E_{33}E_{11}$
$I_E' = E_{33}$
$II_E' = E_{31}^2 + E_{32}^2$

To derive the 2nd Piola-Kirchhoff stress tensor the following relation is used:

$$S_{ij} = \frac{1}{2}\,(\frac{\partial W}{\partial E_{ij}} + \frac{\partial W}{\partial E_{ji}}) \tag{A.6}$$

$$\begin{aligned} S_{ij} = \; & \frac{1}{2}\;\frac{\partial W}{\partial(I_E)}\left(\frac{\partial(I_E)}{\partial E_{ij}} + \frac{\partial(I_E)}{\partial E_{ji}}\right) + \frac{1}{2}\,\frac{\partial W}{\partial(II_E)}\left(\frac{\partial(II_E)}{\partial E_{ij}} + \frac{\partial(II_E)}{\partial E_{ji}}\right) \\ & + \; \frac{1}{2}\,\frac{\partial W}{\partial(I_E')}\left(\frac{\partial(I_E')}{\partial E_{ij}} + \frac{\partial(I_E')}{\partial E_{ji}}\right) + \frac{1}{2}\,\frac{\partial W}{\partial(II_E')}\left(\frac{\partial(II_E')}{\partial E_{ij}} + \frac{\partial(II_E')}{\partial E_{ji}}\right) \end{aligned} \tag{A.7}$$

The derivates of the invariants to the Cauchy-Green strain tensor are:

$$\frac{1}{2}\left(\frac{\partial(I_E)}{\partial E_{ij}}+\frac{\partial(I_E)}{\partial E_{ji}}\right)=\frac{\partial(I_E)}{\partial \mathcal{E}}=\mathcal{I} \tag{A.8}$$

$$\frac{1}{2}\left(\frac{\partial(II_E)}{\partial E_{ij}}+\frac{\partial(II_E)}{\partial E_{ji}}\right)=\mathcal{E}-J_1\,\mathcal{I} \tag{A.9}$$

$$\frac{1}{2}\left(\frac{\partial(I'_E)}{\partial E_{ij}}+\frac{\partial(I'_E)}{\partial E_{ji}}\right)=\frac{\partial(I'_E)}{\partial \mathcal{E}}=\begin{pmatrix}0&0&0\\0&0&0\\0&0&1\end{pmatrix} \tag{A.10}$$

$$\frac{1}{2}\left(\frac{\partial(II'_E)}{\partial E_{ij}}+\frac{\partial(II'_E)}{\partial E_{ji}}\right)=\begin{pmatrix}0&0&E_{13}\\0&0&E_{23}\\E_{31}&E_{32}&0\end{pmatrix} \tag{A.11}$$

Assuming that $a_1 = 2\ a_2 = a_3 = a$, it is now possible to derive the 2nd Piola-Kirchhoff stress tensor:

$$\begin{aligned}\mathcal{S}= \;& W(\mathcal{E}) \quad 2aI_E\mathcal{I}+2aW(\mathcal{E})[\mathcal{E}-I_E\mathcal{I}]+2aW(\mathcal{E})E_{33}\\ &+\quad 2a_4W(\mathcal{E})[E_{31}+E_{13}+E_{32}+E_{23}]\end{aligned} \tag{A.12}$$

Or in matrix notation:

$$\mathcal{S}=2aW(\mathcal{E})\begin{pmatrix}E_{11}&E_{12}&E_{13}\\E_{21}&E_{22}&E_{23}\\E_{31}&E_{32}&E_{33}\end{pmatrix}+a_4W(\mathcal{E})\begin{pmatrix}0&0&E_{13}\\0&0&E_{23}\\E_{31}&E_{32}&0\end{pmatrix} \tag{A.13}$$

A.3 Huyghe

Huyghe specified the strain-energy function by:

$$\begin{aligned}W(\mathcal{E})=\;& c_n\quad \{exp\,(a_{cf}E_{11})-a_{cf}E_{11}+exp\,(a_{cf}E_{22})-a_{cf}E_{22}+exp\,(a_fE_{33})-a_fE_{33}\\ &+\quad [exp\,(a_bE_{11})-a_bE_{11}]\,[exp\,(a_bE_{22})-a_bE_{22}]\\ &+\quad [exp\,(a_bE_{11})-a_bE_{11}]\,[exp\,(a_bE_{33})-a_bE_{33}]\\ &+\quad [exp\,(a_bE_{22})-a_bE_{22}]\,[exp\,(a_bE_{33})-a_bE_{33}]\;-6\}\\ &+\quad c_s\{exp\,[a_s(E_{12}E_{12}+E_{13}E_{13}+E_{23}E_{23})]-1\}\end{aligned} \tag{A.14}$$

This equation can be written as:

$$
\begin{aligned}
W(\mathcal{E}) &= c_n\{exp\,(a_{cf}E_{11}) - a_{cf}E_{11} + exp\,(a_{cf}E_{22}) - a_{cf}E_{22} + exp\,(a_fE_{33}) - a_fE_{33} \\
&+ exp\,(a_bE_{11} + a_bE_{22}) - a_bE_{11}exp\,(a_bE_{22}) - a_bE_{22}exp\,(a_bE_{11}) + a_b^2E_{11}E_{22} \\
&+ exp\,(a_bE_{11} + a_bE_{33}) - a_bE_{33}exp\,(a_bE_{11}) - a_bE_{11}exp\,(a_bE_{33}) + a_b^2E_{11}E_{33} \\
&+ exp\,(a_bE_{22} + a_bE_{33}) - a_bE_{33}exp\,(a_bE_{22}) - a_bE_{22}exp\,(a_bE_{33}) \\
&+ a_b^2E_{22}E_{33} - 6\} + c_s\{exp\,(a_s(E_{12}E_{12} + E_{13}E_{13} + E_{23}E_{23}) - 1)\} \qquad \text{(A.15)}
\end{aligned}
$$

Using this equation and equation A.6 we obtain:

$$
\begin{aligned}
S_{11} = \left(\frac{\partial W}{\partial E_{11}}\right) &= c_n\{a_{cf}exp\,(a_{cf}E_{11}) - a_{cf} + a_bexp\,(a_bE_{11} + a_bE_{22}) \\
&- a_bexp\,(a_bE_{22}) - a_b^2E_{22}exp\,(a_bE_{11}) + a_b^2E_{22} \\
&+ a_bexp\,(a_bE_{11} + a_bE_{33}) - a_b^2E_{33}exp\,(a_bE_{11}) \\
&- a_bexp\,(a_bE_{33}) + a_b^2E_{33}\} \qquad \text{(A.16)}
\end{aligned}
$$

$$
S_{12} = \frac{1}{2}\left(\frac{\partial W}{\partial E_{12}} + \frac{\partial W}{\partial E_{21}}\right) = \frac{1}{2}c_s\{2a_sE_{12}exp\,(a_s(E_{12}E_{12} + E_{13}E_{13} + E_{23}E_{23}))\} \quad \text{(A.17)}
$$

$$
S_{13} = \frac{1}{2}\left(\frac{\partial W}{\partial E_{13}} + \frac{\partial W}{\partial E_{31}}\right) = \frac{1}{2}c_s\{2a_sE_{13}exp\,(a_s(E_{12}E_{12} + E_{13}E_{13} + E_{23}E_{23}))\} \quad \text{(A.18)}
$$

$$
S_{21} = \frac{1}{2}\left(\frac{\partial W}{\partial E_{21}} + \frac{\partial W}{\partial E_{12}}\right) = S_{12} \qquad \text{(A.19)}
$$

$$
\begin{aligned}
S_{22} = \left(\frac{\partial W}{\partial E_{22}}\right) &= c_n\{a_{cf}exp\,(a_{cf}E_{22}) - a_{cf} + a_bexp\,(a_bE_{11} + a_bE_{22}) \\
&- a_b^2E_{11}exp\,(a_bE_{22}) - a_bexp\,(a_bE_{11}) + a_b^2E_{11} \\
&+ a_bexp\,(a_bE_{22} + a_bE_{33}) - a_b^2E_{33}exp\,(a_bE_{22}) \\
&- a_bexp\,(a_bE_{33}) + a_b^2E_{33}\} \qquad \text{(A.20)}
\end{aligned}
$$

$$
S_{23} = \frac{1}{2}\left(\frac{\partial W}{\partial E_{23}} + \frac{\partial W}{\partial E_{32}}\right) = \frac{1}{2}c_s\{2a_sE_{23}exp\,(a_s(E_{12}E_{12} + E_{13}E_{13} + E_{23}E_{23}))\} \quad \text{(A.21)}
$$

$$
S_{31} = \frac{1}{2}\left(\frac{\partial W}{\partial E_{31}} + \frac{\partial W}{\partial E_{13}}\right) = S_{13} \qquad \text{(A.22)}
$$

$$
S_{32} = \frac{1}{2}\left(\frac{\partial W}{\partial E_{32}} + \frac{\partial W}{\partial E_{23}}\right) = S_{23} \qquad \text{(A.23)}
$$

$$
\begin{aligned}
S_{33} = \left(\frac{\partial W}{\partial E_{33}}\right) &= c_n\{a_{cf}exp\,(a_{cf}E_{33}) - a_{cf} + a_b exp\,(a_b E_{11} + a_b E_{33}) \\
&- a_b exp\,(a_b E_{11}) - a_b^2 E_{11} exp\,(a_b E_{33}) + a_b^2 E_{11} \\
&+ a_b exp\,(a_b E_{22} + a_b E_{33}) - a_b exp\,(a_b E_{22}) \\
&- a_b^2 E_{22} exp\,(a_b E_{33}) + a_b^2 E_{22}\}
\end{aligned}
\qquad (A.24)
$$

This can be written as:

$$
\begin{aligned}
S_{ii} = c_n\{a_{cf}E_{ii} - a_c f + a_b\, exp\,(a_b E_{ii} + E_{jj}) - a_b exp\,(a_b E_{jj}) \quad & i=1 \quad j=2,3 \\
-{a_b}^2 E_{jj} exp\,(a_b E_{ii}) + {a_b}^2 E_{jj}\} \quad & i=2 \quad j=1,3 \\
& i=3 \quad j=1,2
\end{aligned}
\qquad (A.25)
$$

$$
S_{ij} = \tfrac{1}{2}c_s\{2a_s E_{ij} exp\,(a_s(E_{12}E_{12} + E_{13}E_{13} + E_{23}E_{23}))\} \qquad i,j = 1,2,3 \quad i \neq j
$$