

THEORETICAL AND NUMERICAL ASPECTS REGARDING THE THERMOELASTIC BEHAVIOUR OF RUBBERLIKE POLYMERS

M.Sc. Szüle V.¹,

Department of Applied Mechanics – University of Széchenyi István, Győr, Hungary
szule.veronika@sze.hu

Abstract: Vehicle components made of rubber usually exhibit large deformations. Cyclic finite deformations may induce increasing temperature in hyperelastic materials. This case - where changes in deformation and in temperature occur simultaneously - is called coupled thermomechanical problem. Both the mechanical and thermal processes have their own governing equations, that is why special techniques are needed for the computation. A special technique will be presented for solving coupled problems, this is operator split method. The goal of this paper is to show how to solve the coupled thermomechanical problem by the principle of virtual power and the principle of virtual temperature, and how to apply them together.

Keywords: RUBBER, HIGH DEFORMATIONS, THERMODYNAMICS

1. Introduction

Rubber can be classified as a so-called hyperelastic polymer which has a typical geometrical and material nonlinear behavior. It means that the relationship between displacements and internal forces can be described by functions whose order is higher than linear. The geometrical nonlinearity is easy to handle mathematically, however the material nonlinearity is only described approximately [1], [2]. Independently of the experimental investigations which deal with the material behavior of rubber, a number of theoretical works treated rubber as an ideally nonlinear elastic, in particular hyperelastic material. One of the properties of the constitutive equations of hyper-elastic material is that stresses are derived from stored elastic energy function. Hyper-elasticity can be described by particularly convenient constitutive equation given its simplicity and it constitutes the basis for more complex material models such as elastoplasticity, viscoplasticity, and viscoelasticity [1].

Furthermore, the task becomes more complicated because of some features of rubber parts. The temperature of rubber increases significantly. Therefore, the temperature- and displacement fields are coupled, and it means that special solving algorithms are required [7]. So the equations of mechanics and thermodynamics are coupled. As described above, the goals of this paper are the following:

It is necessary to summarize the applied equations and the basic physical laws which are responsible for the theoretical background [8,9]. Clarification of these relationships is essential because the material laws of rubber cannot violate those basic physical laws. It is necessary to extend these relationships like balance of linear momentum and balance of angular momentum, the first and second law of thermodynamics to high deformation of rubber and rubberlike polymers. After this, it will follow the solution of the mechanical and heat conduction problem and the coupled thermomechanical problem by using the operator split method. In this paper, arrows above letters denotes vectors and double underline denotes tensor.

2. Governing equations

2.1 Equilibrium of linear momentum

The differential formulation of the equilibrium of linear momentum in the current configuration is

$$\rho \dot{\underline{\underline{v}}} = \underline{\underline{\sigma}} \cdot \underline{\underline{\nabla}} + \underline{\underline{f}} \quad (1)$$

where ρ is the mass density, $\underline{\underline{v}}$ is the velocity, $\underline{\underline{\sigma}}$ is the Cauchy stress, $\underline{\underline{f}}$ is the volume force.

2.2 Equilibrium of angular momentum

The next equality shows the differential form of the balance of the moments.

$$\underline{\underline{\sigma}} = \underline{\underline{\sigma}}^T \quad (2)$$

2.3 First law of thermodynamics

When deformations repeatedly occur, significant increase in temperature can be observed. The differential form of the first law of thermodynamics is in the current configuration

$$\dot{e} \rho = [-\underline{\underline{\nabla}} \cdot \underline{\underline{q}} + h] + \underline{\underline{\sigma}} \cdot \underline{\underline{l}} \quad (3)$$

where e is the internal energy per unit mass, $\underline{\underline{q}}$ is the heat flux, h is the heat source, $\underline{\underline{l}}$ is the velocity gradient, $\underline{\underline{l}} = \underline{\underline{F}} \cdot \underline{\underline{F}}^{-1}$, $\underline{\underline{l}} = \underline{\underline{v}} \circ \underline{\underline{\nabla}}$.

2.4 Second law of thermodynamics

The behaviour of viscoelastic materials is described by the second law of thermodynamics. The second law of thermodynamics in the current configuration can be written as

$$\eta T \rho \geq -\underline{\underline{\nabla}} \cdot \underline{\underline{q}} + \frac{\underline{\underline{q}} \cdot \underline{\underline{\nabla}} T}{T} + h \quad (4)$$

where η is the entropy per unit mass and T is the absolute temperature. It will be practical to change the variable from entropy per unit mass to temperature by applying the Legendre transformation and by using the Helmholtz-free energy

$$\psi = e - \eta T \quad (5)$$

Substitute the Eqn. (5) into to the Eqn. (3) and subtract Eqn. (3) from Eqn. (4) the following expression will be generated

$$-(\dot{\psi} + \eta \dot{T}) \rho + \underline{\underline{\sigma}} \cdot \underline{\underline{l}} - \frac{\underline{\underline{q}} \cdot \underline{\underline{\nabla}} T}{T} - D \geq 0 \quad (6)$$

which is known as Clausius-Duhem inequality [2].

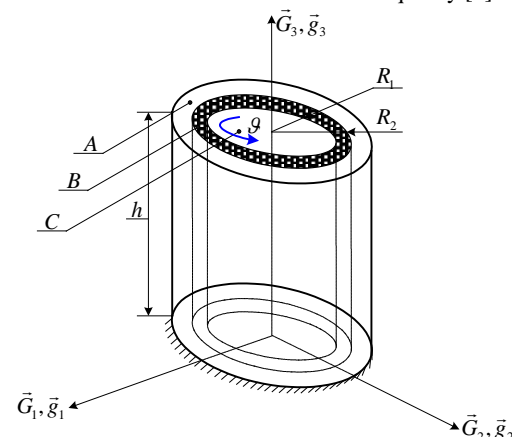


Fig. 1. Mechanical model of a silent block

3. Solution of the coupled thermomechanical problem

3.1 Principle of virtual power

Eq. (1) can be generated in the following form:

$$\underline{\underline{\sigma}} \cdot \nabla + \vec{f} = \vec{0} \quad (7)$$

The solution of Eq. (15) can be generated by finite element method. The basis of the finite element method is an energetical principle, in this case this is the principle of virtual power [4,7].

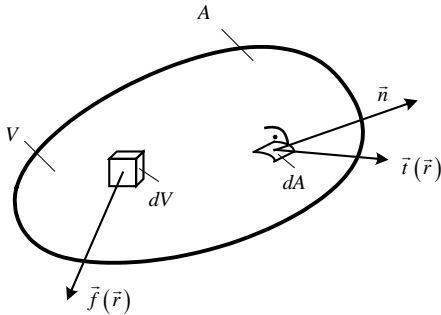


Fig. 2. Types of loads: \vec{t} traction, \vec{f} force per unit volume

Multiplying both sides of Eq. (7) by function \vec{v}^* and integrating the following form will be generated:

$$\int_{(v)} \vec{v}^* \cdot \underline{\underline{\sigma}} \cdot \nabla dv + \int_{(v)} \vec{v}^* \cdot \vec{f} dv = 0 \quad (8)$$

where \vec{v}^* is called virtual velocity field, which is the difference of two different kinematically admissible velocity field and has the following properties: continuous and it can be derivated at least once. The arrow placed above the Cauchy-stress tensor denotes the effect of the Hamiltonian differential operator. Using the $\vec{v}^* \cdot \underline{\underline{\sigma}} \cdot \nabla = \vec{v}^* \cdot \underline{\underline{\sigma}} \cdot \nabla + \vec{v}^* \cdot \underline{\underline{\sigma}} \cdot \nabla$ identity the next expression is generated:

$$\int_{(v)} \vec{v}^* \cdot \underline{\underline{\sigma}} \cdot \nabla dv - \int_{(v)} \vec{v}^* \cdot \underline{\underline{\sigma}} \cdot \nabla dv + \int_{(v)} \vec{v}^* \cdot \vec{f} dv = 0 \quad (9)$$

The first member of Eq. (9) can be converted by Gauss's theorem and the second member can be converted by the application of $\vec{v}^* \cdot \underline{\underline{\sigma}} \cdot \nabla = \underline{\underline{\sigma}} \cdot (\vec{v}^* \circ \nabla)$ identity, where two point means a scalar multiplication between tensors, therefore Eq. (9) results in the following form:

$$\int_{(v)} \vec{v}^* \cdot \underline{\underline{\sigma}} \cdot \vec{n} da - \int_{(v)} \underline{\underline{\sigma}} \cdot (\vec{v}^* \circ \nabla) dv + \int_{(v)} \vec{v}^* \cdot \vec{f} dv = 0$$

The above equation refers to the current configuration so the integration has to be done on the deformed shape of the body. It will be expedient to convert this equation to the reference configuration. Due to this transformation the integrations refer to the undeformable shape of the body.

Let us consider a hyperelastic continuum body in the reference configuration, its volume is indicated by V and its surface is indicated by A . It is known that dv can be expressed by dV

$$dv = JdV \quad (10)$$

and the connection between the surfaces da and dA can be expressed by the Nanson-formula [2]

$$\vec{n} da = J \underline{\underline{F}}^{-T} \cdot \vec{N} dA \quad (11)$$

where $\underline{\underline{F}}^{-T}$ is the inverse of the transpose of the deformation gradient, \vec{N} is the normal vector of surface A , J is the determinant of the deformation gradient. Applying of Eq. (10) and Eq. (11) the Eq. (9) can be obtained, as it can be seen in the next expression:

$$\int_{(A)} \vec{v}^* \cdot \underline{\underline{\sigma}} \cdot \underline{\underline{F}}^{-T} \cdot \vec{N} J dA - \int_{(V)} J \underline{\underline{\sigma}} \cdot (\vec{v}^* \circ \nabla) dV + \int_{(V)} J \vec{v}^* \cdot \vec{f} dV = 0 \quad (12)$$

where $\underline{\underline{P}} = J \underline{\underline{\sigma}} \cdot \underline{\underline{F}}^{-T}$ is the first Piola-Kirchoff stress tensor. The first Piola-Kirchoff stress tensor does not refer to the reference configuration thus it needs to be converted. Multiplying the first member of the left side of Eq. (12) by the $\underline{\underline{I}} = \underline{\underline{F}} \cdot \underline{\underline{F}}^{-1}$ identity tensor and using the $\nabla = \nabla_0 \cdot \underline{\underline{F}}^{-1}$ expression, the following equation will be generated:

$$\int_{(A)} \vec{v}^* \cdot \underline{\underline{F}} \cdot \underline{\underline{F}}^{-1} \cdot \underline{\underline{P}} \cdot \vec{N} dA - \int_{(V)} J \underline{\underline{\sigma}} \cdot (\vec{v}^* \circ \nabla_0) \cdot \underline{\underline{F}}^{-1} dV + \int_{(V)} \vec{v}^* \cdot \vec{f} J dV = 0 \quad (13)$$

where $\underline{\underline{S}}$ is the second Piola-Kirchoff stress tensor which refers to the reference configuration. The surface of the considered body A can be divided into two parts, namely A_u surface where the displacement is defined and A_p where the traction is defined.

The $\underline{\underline{S}} \cdot \vec{N}$ product determines the value of \vec{p}_0 which is the traction vector in the reference configuration. Rearranging the second term of the left side of Eq. (13) the first Piola-Kirchoff stress tensor can be appeared:

$$\int_{(A_p)} \vec{v}^* \cdot \underline{\underline{F}} \cdot \underline{\underline{S}} \cdot \vec{N} dA + \int_{(A_u)} \vec{v}^* \cdot \underline{\underline{F}} \cdot \underline{\underline{S}} \cdot \vec{N} dA - \int_{(V)} J \underline{\underline{\sigma}} \cdot \underline{\underline{F}}^{-T} \cdot (\vec{v}^* \circ \nabla_0) dV + \int_{(V)} \vec{v}^* \cdot \vec{f} J dV = 0 \quad (14)$$

which can be transformed to the second Piola-Kirchoff stress tensor applying the $\underline{\underline{I}} = \underline{\underline{F}} \cdot \underline{\underline{F}}^{-1}$ expression:

$$\int_{(A_p)} \vec{v}^* \cdot \underline{\underline{F}} \cdot \vec{p}_0 dA + \int_{(A_u)} \vec{v}^* \cdot \underline{\underline{F}} \cdot \underline{\underline{S}} \cdot \vec{N} dA - \int_{(V)} \underline{\underline{F}} \cdot \underline{\underline{F}}^{-1} \cdot \underline{\underline{P}} \cdot (\vec{v}^* \circ \nabla_0) dV + \int_{(V)} \vec{v}^* \cdot \vec{f} J dV = 0 \quad (15)$$

The members of this equation can be divided into two groups: virtual power of internal forces (P_{int}) and virtual power of external forces (P_{ext}).

$$P = \int_{(V)} \underline{\underline{S}} \cdot \underline{\underline{F}}^T \cdot (\vec{v}^* \circ \nabla_0) \cdot \underline{\underline{F}} dV - \left(\int_{(A_p)} \vec{v}^* \cdot \underline{\underline{F}} \cdot \vec{p}_0 dA + \int_{(A_u)} \vec{v}^* \cdot \underline{\underline{F}} \cdot \underline{\underline{S}} \cdot \vec{N} dA + \int_{(V)} \vec{v}^* \cdot \vec{f} J dV \right) = 0 \quad (16)$$

Thus the virtual power of internal forces is equivalent the virtual power of external forces [1,2,9].

$$\int_{(V)} \underbrace{\underline{S} \cdot \underline{F}^T \cdot (\underline{v}^* \circ \nabla_0)}_{\underline{r}_{int}} \cdot \underline{F} dV = \int_{(A_p)} \underline{v}^* \cdot \underline{F} \cdot \underline{p}_0 dA + \int_{(A_n)} \underline{v}^* \cdot \underline{F} \cdot \underline{S} \cdot \underline{N} dA + \int_{(V)} \underline{v}^* \cdot \underline{f}_0 dV \tag{17}$$

Denoting by P the difference of the two virtual power, P is the function of the position vector \underline{r} , the function \underline{v}^* and the temperature T due to the thermal expansion.

$$P = P(\underline{r}, T, \underline{v}^*) \tag{18}$$

The thermal expansion is denoted by the next differential equation:

$$\frac{\partial J}{\partial T} = 3\alpha_0 J \tag{19}$$

where α_0 is the linear thermal expansion coefficient. Assuming that the temperature variations are not significant ($T - T_0 \ll T_0$, where T_0 is the reference temperature), the linear thermal expansion coefficient can be considered constant and in that case the solution of Eq. (19) can be determined by the next expression [2]:

$$J(T) = e^{3\alpha_0(T-T_0)} \tag{20}$$

Searching the vector field $\underline{r} = \underline{r}(\underline{R})$ (deformed body) which satisfies the nonlinear equation. Assuming that the mechanical processes are quasi-static processes thus the considered system is in a mechanical equilibrium in each time moment. It means that the acceleration of the points of the continuum body can be assumed zero and the other quantities do not depend on time. Since equation $P = 0$ is nonlinear the solution is generated by Newton-Raphson method:

$$P(\underline{r}_k, \underline{v}^*) + DP(\underline{r}_k, \underline{v}^*)[\underline{u}] = 0 \tag{21}$$

where \underline{r}_k ($k=0$) is an arbitrary vector, $DP(\underline{r}_k, \underline{v}^*)$ is the Gateaux-derivative [1] and \underline{u} is the increment of displacement. After k th iteration steps

$$\underline{r}_{k+1} = \underline{r}_k + \underline{u} \tag{22}$$

the iteration will be stopped when the increment of displacement \underline{u} decreases under the certain margin of error:

$$\frac{|\underline{u}|}{|\underline{r}_k - \underline{R}|} < h \tag{23}$$

3.2 Principle of virtual temperature

In order to solve the coupled thermomechanical problem, it is necessary to solve the heat conduction equation, too [7]. Considering an elastic element which has the property that the total mechanical energy is reversible. The free energy of the body is the function of the strain and temperature. Dissipation comes only from heat conduction.

Starting from the first law of thermodynamics Eq. (8) and changing the variable from entropy to temperature by using the following

expressions: $e = \psi + \eta T$, $\dot{e} = \dot{\psi} + \dot{\eta} T + \eta \dot{T}$, $\psi = \psi(T, \underline{E})$, $\eta = -\frac{\partial \psi}{\partial T}$

$\eta = -\frac{\partial^2 \psi}{\partial T^2} \dot{T} - \frac{\partial^2 \psi}{\partial T \partial \underline{E}} \cdot \underline{\dot{E}}$ the equation of heat conduction in the reference configuration is

$$\rho_0 c \dot{T} = -\nabla_0 \cdot \underline{\bar{q}}_0 + h_0 + \left(\underline{S} - \rho_0 \frac{\partial \psi}{\partial \underline{E}} + \rho_0 T \frac{\partial^2 \psi}{\partial \underline{E} \partial T} \right) \cdot \underline{\dot{E}} \tag{24}$$

where ρ_0 is the mass density in the reference configuration, c is

the heat capacity, $\underline{\bar{q}}_0$ is the heat flux vector in the reference configuration, h_0 is the heat source, where \underline{E} is the Green-Lagrange strain tensor. Correspondingly, the mechanical equation of the heat conduction equation can be solved by finite element method. The solution can be determined by the principle of virtual temperature. Assuming that the considered material is perfectly elastic the non-recoverable part of the mechanical power is:

$$\underline{S} - \rho_0 \frac{\partial \psi}{\partial \underline{E}} = \underline{0} \tag{25}$$

Thus, the equation of heat conduction can be generated in the following form:

$$\rho_0 c \dot{T} = -\nabla_0 \cdot \underline{\bar{q}}_0 + h_0 + \rho_0 T \frac{\partial^2 \psi}{\partial \underline{E} \partial T} \cdot \underline{\dot{E}} \tag{26}$$

Multiplying both sides of Eq. (26) by function $\theta(\underline{r}, t)$ and integrating both sides, the following form will be generated:

$$\int_{(V)} \rho_0 c \dot{T} \theta dV = - \int_{(V)} \nabla_0 \cdot \underline{\bar{q}}_0 \theta dV + \int_{(V)} h_0 \theta dV + \int_{(V)} \rho_0 T \frac{\partial^2 \psi}{\partial \underline{E} \partial T} \cdot \underline{\dot{E}} \theta dV \tag{27}$$

where is $\theta(\underline{r}, t)$ called virtual temperature field, which has the similar properties

such as virtual velocity field, so it is continuous and it can be derivated at least once. Consequence of the second law of thermodynamics is that the heat flux can be expressed by the negative gradient of the temperature field [7]:

$$\underline{\bar{q}}_0 = -\underline{\kappa} \cdot \nabla_0 T \tag{28}$$

where $\underline{\kappa}$ is the heat conduction tensor. Applying Gauss's theorem:

$$\int_{(V)} \rho_0 c \dot{T} \theta dV = - \int_{(A)} \theta \underline{\bar{q}}_0 \cdot \underline{N} dA - \int_{(V)} \theta \nabla_0 \cdot \underline{\kappa} \cdot \nabla_0 T dV + \int_{(V)} h_0 \theta dV + \int_{(V)} \rho_0 T \frac{\partial^2 \psi}{\partial \underline{E} \partial T} \cdot \underline{\dot{E}} \theta dV \tag{29}$$

Considering that the surface of the body can be divided according to the boundary conditions into two parts, the first member of the right side of Eq. (29) consists of two parts. The first part is the integral on the surface A_T where the temperature is given, the second is the integral on the surface A_q where the heat flux is given, as is presented in Fig. 3.

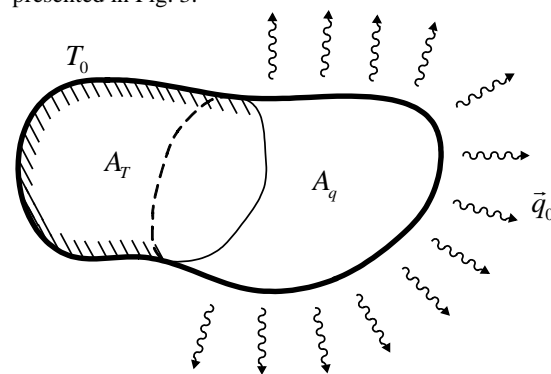


Fig. 3. Boundary conditions: defined temperature, defined heat flux

Furthermore, assuming that the considered material is isotrop in respect of heat conduction, thus $\underline{\kappa} = \kappa \underline{I}$, where \underline{I} denotes the identity tensor, the equation of heat conduction will have the next form:

$$\int_{(V)} \rho_0 c \dot{T} \theta dV = \int_{(A_r)} \kappa \theta (\nabla_0 T) \cdot \vec{N} dA - \int_{(A_s)} \theta \underbrace{\vec{q}_0}_{q_N} \cdot \vec{N} dA - \int_{(V)} \kappa (\theta \nabla_0) \cdot (\nabla_0 T) dV + \int_{(V)} h_0 \theta dV + \int_{(V)} \rho_0 T \frac{\partial^2 \psi}{\partial \underline{E} \partial T} \cdot \underline{E} \theta dV \quad (30)$$

Directing Eq. (30) to zero, the principle of virtual temperature can be determined which can be used for the approximate solution of the differential equation Eq. (26)

$$\begin{aligned} \Upsilon = \int_{(V)} \rho_0 c \dot{T} \theta dV + \int_{(A)} \theta q_N dA + \int_{(V)} \kappa \theta \nabla_0 \cdot \nabla_0 T dV - \\ - \int_{(V)} h_0 \theta dV - \int_{(V)} \rho_0 T \frac{\partial^2 \psi}{\partial \underline{E} \partial T} \cdot \underline{E} \theta dV = 0 \end{aligned} \quad (31)$$

where Υ is function of the \vec{r} position vector, the θ function and the T temperature, $\Upsilon = \Upsilon(\vec{r}, T, \theta)$. Searching the temperature field $T(\vec{r}, t)$ which satisfies the equation $\Upsilon = 0$.

3.3 Solution of the coupled thermomechanical problem

For the solution of the coupled problem, a special technique will be presented which is called operator split method. The solution is divided into two parts by the above mentioned method. First of all, the mechanical problem has to be solved with constant temperature:

$$P = P(\vec{r}, T = \text{const.}, \vec{v}^*) = 0 \quad (32)$$

The result of Eq. (32) is the \vec{r} function. It will be followed by the solution of the heat conduction problem with constant \vec{r} function, in the following manner:

$$\Upsilon = \Upsilon(\vec{r} = \text{const.}, T, \theta) = 0 \quad (33)$$

Substituting the resulted temperature field into the mechanical equation, the mechanical equation has to be solved again. These above mentioned two steps have to be repeated till the variation of the \vec{r} function and temperature decrease under these margin of errors:

$$\frac{|\vec{r}_k - \vec{r}_{k-1}|}{|\vec{r}_k - \vec{R}|} < h_1 \quad (34)$$

and

$$\frac{|T_k - T_{k-1}|}{|T_k - T_0|} < h_2 \quad (35)$$

where h_1 and h_2 are margins of errors and T_0 is the reference temperature.

In order to solve the thermomechanical problem, it is necessary to use the weak formulation and to do the linearization of the non-linear formulation of the mechanical problem. The position vector is determined from the weak form of the mechanical problem, the temperature field is determined from the weak form of the heat conduction problem. The flowchart of the numerical solution is presented in Fig. 4.

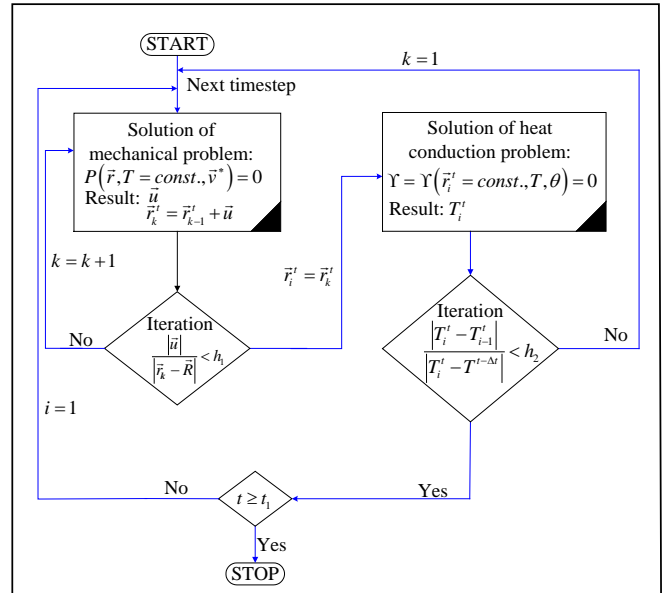


Fig. 4. Flowchart of solution of the coupled thermomechanical problem

4. Summary

We represented an algorithm which allows to calculate strain changes and temperature changes of the rubber part of a vehicle component under certain conditions. In the future we would like to develop a solving computer program in order to apply it as a thermodynamically consistent description.

The present numerical algorithm is the basis of the further fatigue and lifetime-calculations.

References

- [1] Bonet, J., Wood, R. D.: Nonlinear Continuum Mechanics for Finite Element Analysis, Cambridge University Press (1997).
- [2] Holzapfel, G. A.: Nonlinear Solid Mechanics, John Wiley&Sons, Chichester, (2000).
- [3] Ogden, R. W., Large deformation isotropic elasticity: on the correlation of theory and experiment for incompressible rubberlike solids, Proc. Royal Society of London, Series A 326, pp. 565-584. (1972)
- [4] Ogden, R. W., Elastic deformations of rubberlike materials, H.G.Hopkins and M.J. Sewell, eds., Mechanics of Solids, the Rodney Hill 60th Anniversary Volume, (Pergamon Press, Oxford), pp. 499-537, (1982).
- [5] Reese S., Wriggers P.: A material model for rubber-like polymers exhibiting plastic deformation: computational aspects and a comparison with experimental results, Computer methods in applied mechanics and engineering, Vol 148, pp. 279-298, (1997).
- [6] Böl, M., Reese, S.: Finite element modelling of rubber-like polymers based on chain statistics, International Journal of Solids and Structures, Vol 43, pp. 2-26, (2006).
- [7] Pere, B.: Solution of Coupled Thermomechanical Problems Using p-FEM, 8th European Solid Mechanics Conference (ESMC2012), (CD-ROM, 2 pages), Graz, Austria, 9-13 July (2012).
- [8] Holzapfel, G. A., Simo J., C.: Entropy elasticity of isotropic rubber-like solids at finite strains, Computer methods in applied mechanics and engineering, Vol 132, pp. 17-44. (1996).
- [9] Égert J., Pere B.: Finite Element Analysis, Universitas Győr Nonprofit Kft., Hungary, Győr (2011).