Simulation of Thermomechanical Couplings of Viscoelastic Materials

Frank Neff[1], Thomas Miquel[2], Michael Johlitz[1], Alexander Lion[1]

[1]Institute of Mechanics
Faculty for Aerospace Engineering
Universität der Bundeswehr München
[2]École Polytechnique, Paris

October, 14th 2016

COMSOL CONFERENCE 2016 MUNICH

Universität der Bundeswehr München

Contents

Contents

Motivation

Technical applications of elastomers, e.g.

- bearings
- tires
- sealings
- etc.

CSR New Material Technologies GmbH

Motivation

Technical applications of elastomers, e.g.

- bearings
- tires
- sealings
- etc.

CSR New Material Technologies GmbH

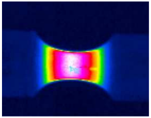
Properties of elastomers

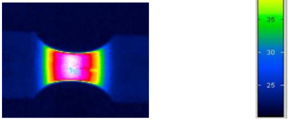
- viscoelastic material behaviour
- glass transition
- aging (physical, chemical)
- Mullins-Effect
- Payne-Effect
- self-heating
- swelling

www.citoen-L-attraction.de

Self-heating

- dynamic mechanical loads and finite strains
- energy dissipation causes increase in temperature





Self-heating

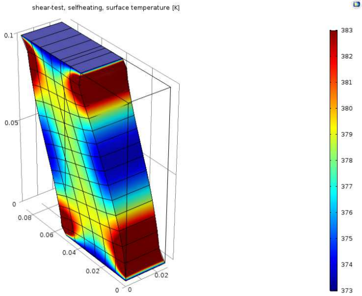
- dynamic mechanical loads and finite strains
- energy dissipation causes increase in temperature

Need to consider self-heating

- temperature influences the whole stress-strain relation
- dynamic mechanical loads cause change in temperature
- complex structures exhibit a complex temperature field

Challenges

- finite viscoelastic material behaviour (isothermal)
- coupling between dissipated energy and temperature
- temperature dependent change of material parameters
- time efficient computation



Shear test 3d

Challenges

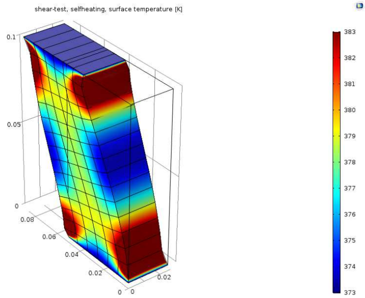
- finite viscoelastic material behaviour (isothermal)
- coupling between dissipated energy and temperature
- temperature dependent change of material parameters
- time efficient computation

Our contributions

- model for non-linear viscoelastic materials
- model for heat transfer
- multiphysics coupling thermal expansion
- multiphysics coupling dissipation

following:

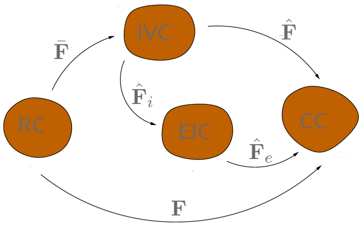
- Johlitz 2015
- Dippel 2015
- Dippel and Johlitz 2014



Shear test 3d

Contents

Deformation Gradient $\mathbf{F}$

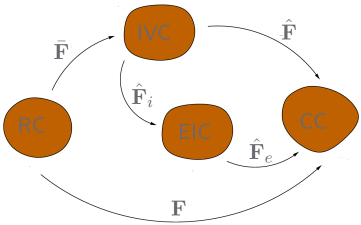


(Johlitz, Dippel, and Lion 2015)

Separate volumetric and isocoric deformation

- volumetric deformation $\bar{\mathbf{F}}$ due to thermal expansion
- elastomers are considered as nearly incompressible referring to mechanical loads
- isochoric deformation $\hat{\mathbf{F}}$ due to mechanical loadings
- multiplicative split of the deformation gradient (Lee 1969)
  $\mathbf{F} = \hat{\mathbf{F}} \cdot \bar{\mathbf{F}}$

Deformation Gradient $\mathbf{F}$



(Johlitz, Dippel, and Lion 2015)

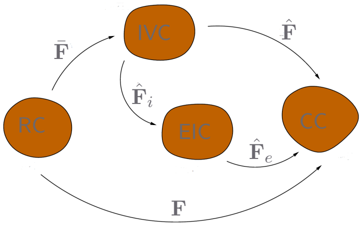
Separate volumetric and isocoric deformation

- volumetric deformation $\bar{\mathbf{F}}$ due to thermal expansion
- elastomers are considered as nearly incompressible referring to mechanical loads
- isochoric deformation $\hat{\mathbf{F}}$ due to mechanical loadings
- multiplicative split of the deformation gradient (Lee 1969)
  $\mathbf{F} = \hat{\mathbf{F}} \cdot \bar{\mathbf{F}}$

Volumetric deformation gradient $\bar{\mathbf{F}}$

- $\bar{\mathbf{F}} = J^{\frac{1}{3}} \mathbf{I}$
- $\det(\bar{\mathbf{F}}) = \alpha\,(\theta - \theta_0)$
- coefficient of thermal expansion α

Deformation Gradient $\mathbf{F}$



(Johlitz, Dippel, and Lion 2015)

Separate volumetric and isocoric deformation

- volumetric deformation $\bar{\mathbf{F}}$ due to thermal expansion
- elastomers are considered as nearly incompressible referring to mechanical loads
- isochoric deformation $\hat{\mathbf{F}}$ due to mechanical loadings
- multiplicative split of the deformation gradient (Lee 1969)
  $\mathbf{F} = \hat{\mathbf{F}} \cdot \bar{\mathbf{F}}$

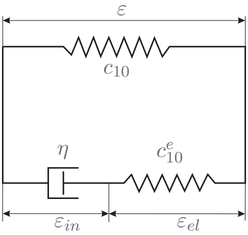
Volumetric deformation gradient $\bar{\mathbf{F}}$

- $\bar{\mathbf{F}} = J^{\frac{1}{3}}\,\mathbf{I}$
- $\det\left(\bar{\mathbf{F}}\right) = \alpha\,(\theta - \theta_0)$
- coefficient of thermal expansion α

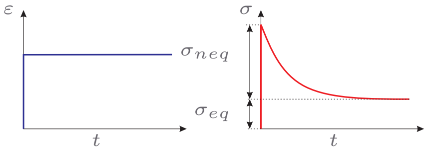
Isochoric deformation gradient $\hat{\mathbf{F}}$

- $\hat{\mathbf{F}} = J^{-\frac{1}{3}}\,\mathbf{F}$
- $\det\left(\hat{\mathbf{F}}\right) = 1$

Finite viscoelasticity



3-parameter-model

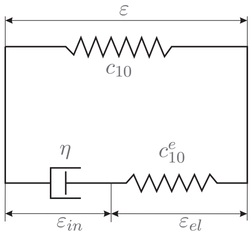


strain-time relation / stress-time relation of the 3-parameter-model

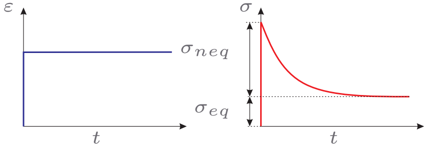
Modelling finite viscoelasticity

- equilibrium spring:
  - hyperelastic material model (e.g. Neo-Hooke)
  - no time dependence
- Maxwell-element:
  - spring is modelled as Neo-Hookean-spring
  - time dependent behaviour of the damper

Finite viscoelasticity



3-parameter-model



strain-time relation / stress-time relation of the 3-parameter-model

Modelling finite viscoelasticity

- equilibrium spring:
  - hyperelastic material model (e.g. Neo-Hooke)
  - no time dependence
- Maxwell-element:
  - spring is modelled as Neo-Hookean-spring
  - time dependent behaviour of the damper

Elastic-inelastic split of $\hat{\mathbf{F}}$

- elastic part $\hat{\mathbf{F}}_e$
- inelastic part $\hat{\mathbf{F}}_i$
- multiplicative split of the isochoric deformation gradient $\hat{\mathbf{F}} = \hat{\mathbf{F}}_e \cdot \hat{\mathbf{F}}_i$

Entropy balance

Clausius-Duhem-Inequality (CDI) (Haupt 2002)

$$-\rho_0 \, \dot{\psi} + \bar{\mathbf{T}} : \dot{\mathbf{E}} - \rho_0 \, s \, \dot{\theta} - \frac{\mathbf{q_0}}{\theta} \cdot \operatorname{Grad} \theta \geq 0$$

- ψ: Helmholtz free energy
- $\bar{\mathbf{T}}$: 2nd Piola-Kirchhoff stress tensor
- $\mathbf{E}$: Green-Lagrangean strain tensor

Entropy balance

Clausius-Duhem-Inequality (CDI) (Haupt 2002)

$$-\rho_0\,\dot{\psi} + \bar{\mathbf{T}} : \dot{\mathbf{E}} - \rho_0\, s\,\dot{\theta} - \frac{\mathbf{q}_0}{\theta} \cdot \mathrm{Grad}\,\theta \geq 0$$

- ψ: Helmholtz free energy
- $\bar{\mathbf{T}}$: 2nd Piola-Kirchhoff stress tensor
- $\mathbf{E}$: Green-Lagrangean strain tensor

Additive formulation of the Helmholtz free energy

$$\psi = \psi_{eq}^{vol}\,(J,\theta) + \psi_{eq}^{iso}\left(\hat{\mathbf{C}}\right) + \psi_{neq}^{iso}\left(\hat{\mathbf{C}}_e\right)$$

Entropy balance

Clausius-Duhem-Inequality (CDI) (Haupt 2002)

$$-\rho_0\,\dot{\psi} + \bar{\mathbf{T}} : \dot{\mathbf{E}} - \rho_0\, s\,\dot{\theta} - \frac{\mathbf{q_0}}{\theta}\cdot \mathrm{Grad}\,\theta \geq 0$$

- ψ: Helmholtz free energy
- $\bar{\mathbf{T}}$: 2nd Piola-Kirchhoff stress tensor
- $\mathbf{E}$: Green-Lagrangean strain tensor

Additive formulation of the Helmholtz free energy

$$\psi = \psi_{eq}^{vol}\left(J,\theta\right) + \psi_{eq}^{iso}\left(\hat{\mathbf{C}}\right) + \psi_{neq}^{iso}\left(\hat{\mathbf{C}}_e\right)$$

Helmholtz free energy and CDI

$$-\left(p + \rho_0\,\frac{\partial\psi_{eq}^{vol}}{\partial J}\right)\dot{J} - \left(\rho_0\,s + \rho_0\,\frac{\partial\psi_{eq}^{vol}}{\partial\theta}\right)\dot{\theta} - \frac{\mathbf{q_0}}{\theta}\cdot \mathrm{Grad}\,\theta +$$
$$\left(\frac{1}{2}\,J\,\hat{\mathbf{T}} - \rho_0\,\frac{\partial\psi_{eq}^{iso}}{\partial\hat{\mathbf{C}}} - \rho_0\,\hat{\mathbf{F}}_i^{-1}\cdot\frac{\partial\psi_{neq}^{iso}}{\partial\hat{\mathbf{C}}_e}\cdot\hat{\mathbf{F}}_i^{-T}\right) : \dot{\hat{\mathbf{C}}} + \rho_0\,\frac{\partial\psi_{neq}^{iso}}{\partial\hat{\mathbf{C}}_e} : \left(\hat{\mathbf{C}}_e\cdot\hat{\mathbf{L}}_i + \hat{\mathbf{L}}_i\cdot\hat{\mathbf{C}}_e\right) \geq 0$$

Material modelling

Approach for Helmholtz free energy density

$$\rho_0\,\psi_{eq}^{vol} = \frac{1}{2}\,K\,\left[(J-1)^2 + (\ln J)^2\right] - K\,\alpha\,(J-1)\,(\theta-\theta_0) - \rho_0\,c(\theta)$$
$$\rho_0\,\psi_{eq}^{iso} = c_{10}\left(\mathrm{I}_{\hat{\mathbf{C}}} - 3\right)$$
$$\rho_0\,\psi_{neq}^{iso} = c_{10}^{e}\left(\mathrm{I}_{\hat{\mathbf{C}}_e} - 3\right)$$

Material modelling

Approach for Helmholtz free energy density

$$\rho_0\,\psi_{eq}^{vol} = \frac{1}{2}\,K\,\left[(J-1)^2 + (\ln J)^2\right] - K\,\alpha\,(J-1)\,(\theta-\theta_0) - \rho_0\,c(\theta)$$

$$\rho_0\,\psi_{eq}^{iso} = c_{10}\left(\mathrm{I}_{\hat{\mathbf{C}}} - 3\right)$$

$$\rho_0\,\psi_{neq}^{iso} = c_{10}^{e}\left(\mathrm{I}_{\hat{\mathbf{C}}_e} - 3\right)$$

Evaluation of the constitutive equations

$$p = -K\left[(J-1) + \frac{\ln J}{J}\right] + K\,\alpha\,(\theta-\theta_0)$$

$$s = \frac{1}{\rho_0}\left(K\,\alpha\,(J-1) + \rho_0\,\frac{\partial c(\theta)}{\partial\theta}\right)$$

$$\hat{\mathbf{T}} = 2\,J^{-1}\,c_{10}\,\mathbf{I} + 2\,J^{-1}\,c_{10}^{e}\,\hat{\mathbf{C}}_i^{-1} - \frac{2}{3}\,J^{-1}\left(c_{10}\,\mathrm{tr}\,\hat{\mathbf{C}} + c_{10}^{e}\,\mathrm{tr}\,\hat{\mathbf{C}}_e\right)\hat{\mathbf{C}}^{-1}$$

Final equations

2nd Piola-Kirchhoff stress tensor

$$\bar{\mathbf{T}} = -p\, J\, \mathbf{C}^{-1} + 2\, J^{-\frac{2}{3}}\, c_{10} \left(\mathbf{I} - \frac{1}{3}\, \mathrm{tr}(\hat{\mathbf{C}})\hat{\mathbf{C}}^{-1} \right) + 2\, J^{-\frac{2}{3}}\, c_{10}^{e} \left(\hat{\mathbf{C}}_i^{-1} - \frac{1}{3}\, \mathrm{tr}\left(\hat{\mathbf{C}}_i^{-1} \cdot \hat{\mathbf{C}} \right) \hat{\mathbf{C}}^{-1} \right)$$

Final equations

2nd Piola-Kirchhoff stress tensor

$$\bar{\mathbf{T}} = -p\, J\, \mathbf{C}^{-1} + 2\, J^{-\frac{2}{3}}\, c_{10} \left(\mathbf{I} - \tfrac{1}{3}\, \mathrm{tr}(\hat{\mathbf{C}})\hat{\mathbf{C}}^{-1} \right) + 2\, J^{-\frac{2}{3}}\, c_{10}^{e} \left(\hat{\mathbf{C}}_i^{-1} - \tfrac{1}{3}\, \mathrm{tr}\left(\hat{\mathbf{C}}_i^{-1} \cdot \hat{\mathbf{C}} \right) \hat{\mathbf{C}}^{-1} \right)$$

Evolution equation

$$\dot{\hat{\mathbf{C}}}_i = \frac{2\, c_{10}^{e}}{\eta(\theta)} \left(\hat{\mathbf{C}} - \tfrac{1}{3}\, \mathrm{tr}\left(\hat{\mathbf{C}} \cdot \hat{\mathbf{C}}_i^{-1} \right) \hat{\mathbf{C}}_i \right)$$

Final equations

2nd Piola-Kirchhoff stress tensor

$$\bar{\mathbf{T}} = -p\, J\, \mathbf{C}^{-1} + 2\, J^{-\frac{2}{3}}\, c_{10} \left(\mathbf{I} - \frac{1}{3}\, \text{tr}(\hat{\mathbf{C}})\hat{\mathbf{C}}^{-1} \right) + 2\, J^{-\frac{2}{3}}\, c_{10}^{e} \left(\hat{\mathbf{C}}_i^{-1} - \frac{1}{3}\, \text{tr}\left(\hat{\mathbf{C}}_i^{-1} \cdot \hat{\mathbf{C}} \right) \hat{\mathbf{C}}^{-1} \right)$$

Evolution equation

$$\dot{\hat{\mathbf{C}}}_i = \frac{2\, c_{10}^{e}}{\eta(\theta)} \left(\hat{\mathbf{C}} - \frac{1}{3}\, \text{tr}\left(\hat{\mathbf{C}} \cdot \hat{\mathbf{C}}_i^{-1} \right) \hat{\mathbf{C}}_i \right)$$

Heat transfer equation

$$K\, \alpha\, \theta\, \dot{J} + \rho_0\, (A + B\, \theta)\, \dot{\theta} - \lambda_\theta\, \text{Div}\,(\text{Grad}\,(\theta)) - c_{10}^{e}\, \hat{\mathbf{C}}_i^{-1} \cdot \hat{\mathbf{C}} \cdot \hat{\mathbf{C}}_i^{-1} : \dot{\hat{\mathbf{C}}}_i = 0$$

Final equations

2nd Piola-Kirchhoff stress tensor

$$\bar{\mathbf{T}} = -p\, J\, \mathbf{C}^{-1} + 2\, J^{-\frac{2}{3}}\, c_{10} \left(\mathbf{I} - \frac{1}{3}\, \mathrm{tr}(\hat{\mathbf{C}})\hat{\mathbf{C}}^{-1} \right) + 2\, J^{-\frac{2}{3}}\, c_{10}^{e} \left(\hat{\mathbf{C}}_i^{-1} - \frac{1}{3}\, \mathrm{tr}\left(\hat{\mathbf{C}}_i^{-1} \cdot \hat{\mathbf{C}} \right) \hat{\mathbf{C}}^{-1} \right)$$

Evolution equation

$$\dot{\hat{\mathbf{C}}}_i = \frac{2\, c_{10}^{e}}{\eta(\theta)} \left(\hat{\mathbf{C}} - \frac{1}{3}\, \mathrm{tr}\left(\hat{\mathbf{C}} \cdot \hat{\mathbf{C}}_i^{-1} \right) \hat{\mathbf{C}}_i \right)$$

Heat transfer equation

$$K\, \alpha\, \theta\, \dot{J} + \rho_0\, (A + B\, \theta)\, \dot{\theta} - \lambda_\theta\, \mathrm{Div}\,(\mathrm{Grad}\,(\theta)) - c_{10}^{e}\, \hat{\mathbf{C}}_i^{-1} \cdot \hat{\mathbf{C}} \cdot \hat{\mathbf{C}}_i^{-1} : \dot{\hat{\mathbf{C}}}_i = 0$$

Williams-Landel-Ferry equation (WLF)

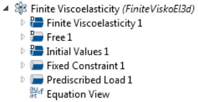
$$\eta(\theta) = \eta_0\, \exp\left(-\frac{C_1\,(\theta - \theta_G)}{C_2 + \theta - \theta_G} \right)$$

Contents

Mechanical behaviour

Physics interface: Finite Viscoelasticity

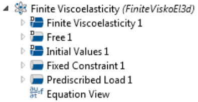
- Domain feature
- Boundary conditions:
  - Fixed Constraint
  - Predescribed Displacement
  - Predescribed Load

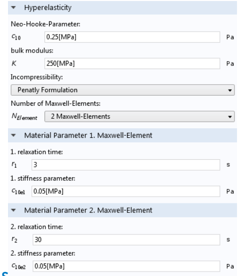


Mechanical behaviour

Physics interface: Finite Viscoelasticity

- Domain feature
- Boundary conditions:
  - Fixed Constraint
  - Predescribed Displacement
  - Predescribed Load





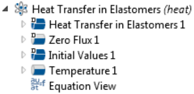
Domain feature: Finite Viscoelasticity 1

- equilibrium part: Neo-Hooke
- incompressibility:
  - Penalty-Formulation
  - Lagrange-Formulation
- number of Maxwell-Elements (0-5)

Thermal behaviour

Physics interface: Heat Transfer

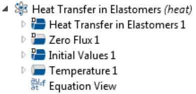
- Domain feature
- Boundary conditions:
  - Temperature
  - Adiabat



Thermal behaviour

Physics interface: Heat Transfer

- Domain feature
- Boundary conditions:
  - Temperature
  - Adiabat



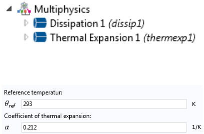
Domain feature: Heat Transfer 1

- Fourier heat transfer

Couplings

Multiphysics coupling: Thermal Expansion

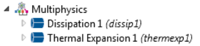
- coupling of:
  - Finite Viscoelasticity
  - Heat-Transfer
- thermal expansion coefficient

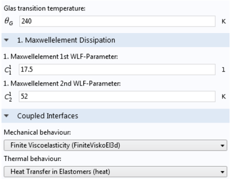


Couplings

Multiphysics coupling: Thermal Expansion

- coupling of:
  - Finite Viscoelasticity
  - Heat-Transfer
- thermal expansion coefficient





Multiphysics coupling: Dissipation

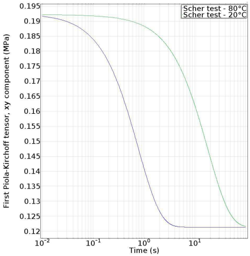
- self-heating
- WLF-Parameters for each Maxwell-Element
- could be combined with thermal expansion

Contents

Temperature influence of viscoelasticity

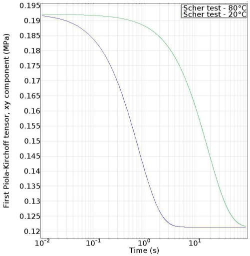
Static shear test

- shear angle 20°
- temperature $293\,\mathrm{K}$ and $363\,\mathrm{K}$
- chosen academic material parameters



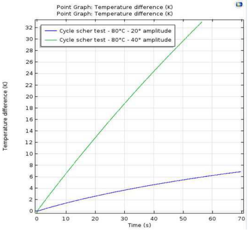
Results

Temperature influence of viscoelasticity



Static shear test

- shear angle 20°
- temperature $293\,\mathrm{K}$ and $363\,\mathrm{K}$
- chosen academic material parameters

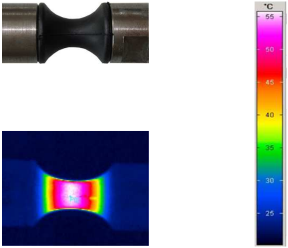


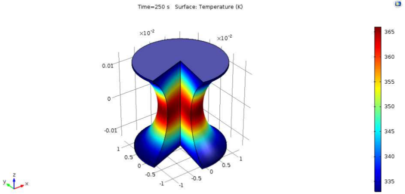
Dynamic shear test

- shear angle 20° and 40° (amplitude)
- sinus cycle with $4\,\mathrm{Hz}$ frequency
- temperature $363\,\mathrm{K}$
- chosen academic material parameters

Results

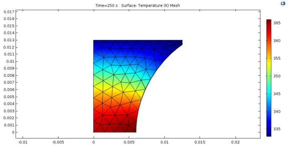
Cyclic deformation of an hourglass sample





Cyclic test of an hourglass sample

- tension 6 mm
- sinus cycle with 4 Hz frequency (tension only)
- temperature 333 K
- chosen academic material parameters
- material parameters could be identified by DMA experiment



Conclusions

- a model for finite viscoelastic material behaviour is proposed and implemented
- temperature dependence of mechanical behaviour is guaranteed by WLF-approach for the relaxation times
- coupling of dissipated mechanical energy and temperature field
- coupling temperature and volumetric expansion
- modular setup leads to flexibility in application

Literature

Dippel, B. (2015).
Experimentelle Charakterisierung, Modellierung und FE-Berechnung thermomechanischer Kopplung.
Ph. D. thesis, Universität der Bundeswehr München.

Dippel, B. and M. Johlitz (2014).
Thermo-mechanical couplings in elastomers - experiments and modelling.
ZAM Zeitschrift für Angewandte Mathematik und Mechanik.

Haupt, P. (2002).
Continuum Mechanics and Theory of Materials.
Springer Verlag.

Johlitz, M., B. Dippel, and A. Lion (2015).
Dissipative heating of elastomers: a new modelling approach based on finite and coupled thermomechanics.
Continuum Mechanics and Thermodynamics, 1–15.

Lee, E. (1969).
Elastic-plastic deformatin at finite strain.
Jounal of Applied Mechanics 36, 1–6.