COMSOL Conference 2016 Munich

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Simulation and numerical implementation of chemo-thermomechanical aging of rubber

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Outline

- Introduction and motivation
- Constitutive modelling approach
- Implementation into COMSOL
- Simulations
- Summary and outlook

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Introduction & motivation

External influences on elastomers in technical applications

temperature

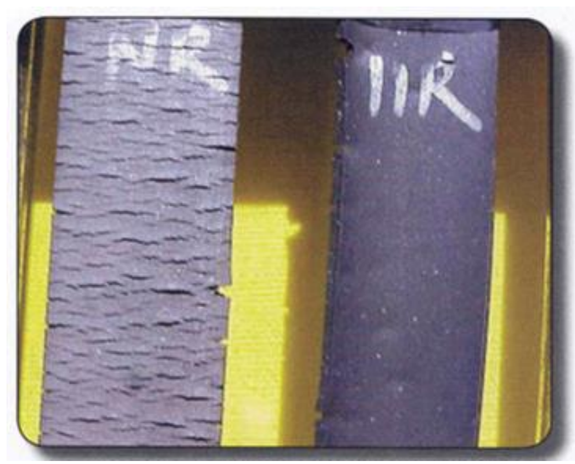
oxygen O_2

moisture

UV

oil

radiation



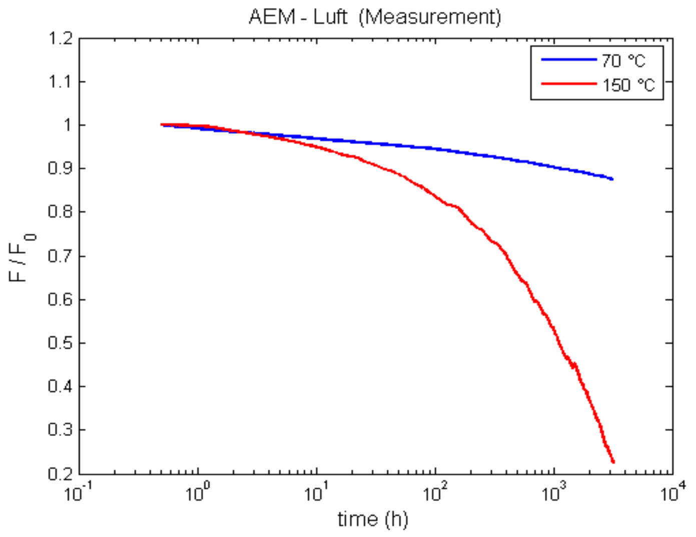
source: www.timcorubber.com

$\vec{F}$ mechanical loads

ozone O_3

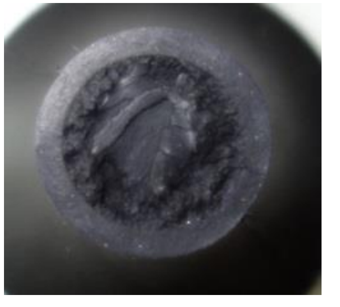
chemicals

Introduction & motivation



Aging induced stress relaxation

Tension/Compression set

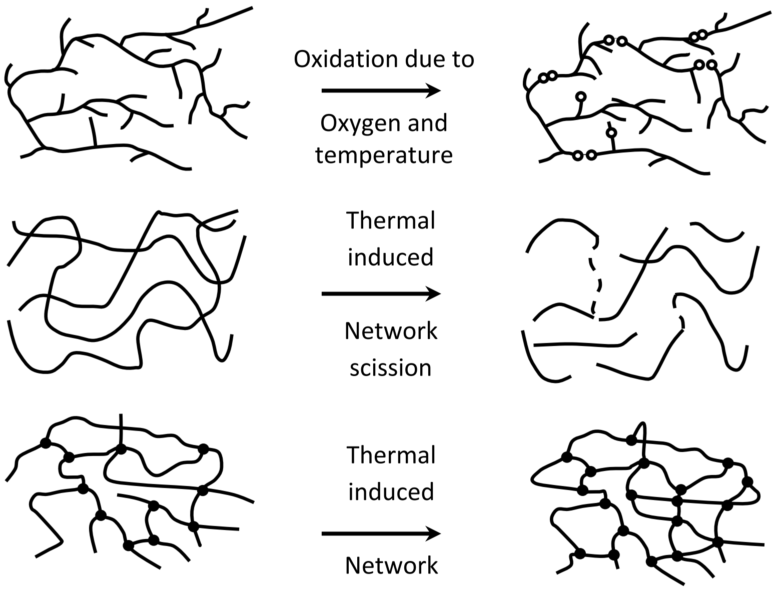


DLO Effect

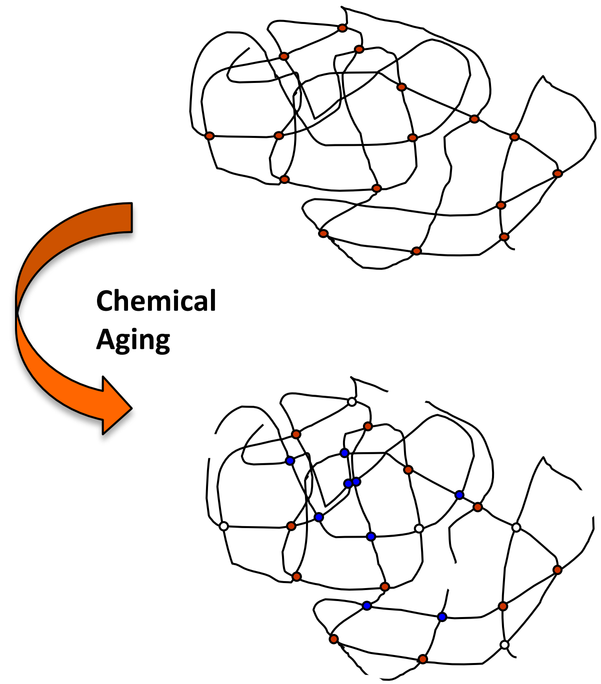
Modell requirements

- Change of mechanical properties due to aging
- Tension/Compression set
- DLO Effect
- Material behavior: nonlinear thermoviscoelasticity

Introduction & motivation



Ehrenstein (2007)



Chemical Aging

- Irreversible chemical change as a result of oxygen diffusion and reaction with the elastomer; elevated temperatures accelerate the aging process
- Degeneration of chemical bonds (**Network-Degradation**)
- Formation of new network junctions (**Network-Reformation**)

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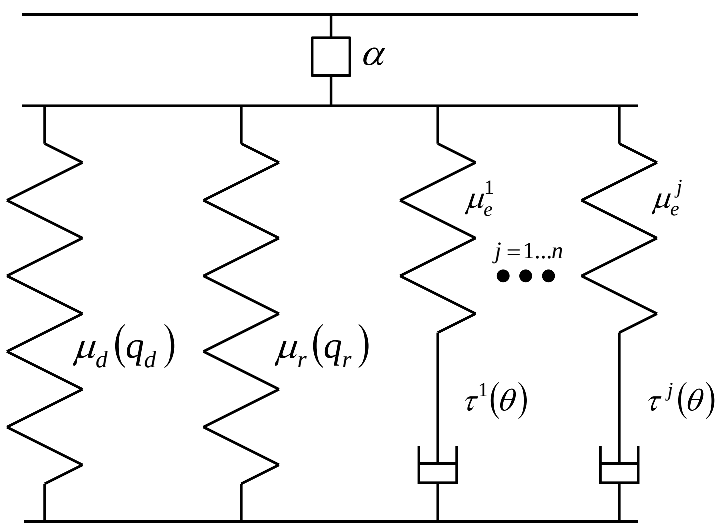
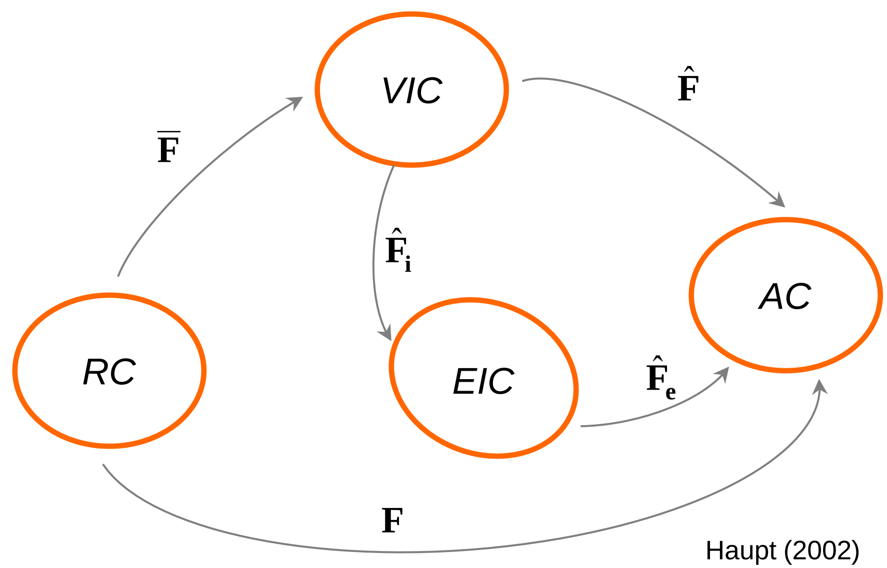
Modelling

- Rheological model (Neo-Hooke)



- General motion of a deformable body



Haupt (2002)

Lion (1996)

- Thermo-mechanical consistence (C.-D. inequality)

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

$$\psi = \psi\left(\hat{\mathbf{C}}, \hat{\mathbf{C}}_e,\ J, \theta, q_d, q_r, c\right) \longrightarrow$$ Helmholz free energy function

Modelling

Set of constitutive eq. and evolution eq. can be evaluated

- Stress (2.PK)

$$\tilde{\mathbf{T}} = \tilde{\mathbf{T}}_{eq}^{VOL} + \tilde{\mathbf{T}}_{d}^{ISO} + \tilde{\mathbf{T}}_{r}^{ISO} + \tilde{\mathbf{T}}_{neq}^{ISO}$$

$$\tilde{\mathbf{T}} = K\left[(J-1) + \ln J / J\right] J\mathbf{C}^{-1} - K\alpha(\theta - \theta_0) J\mathbf{C}^{-1} + \mu_d(q_d) J^{-2/3}\left(\mathbf{1} - \tfrac{1}{3} tr\left(\hat{\mathbf{C}}\right)\hat{\mathbf{C}}^{-1}\right) +$$
$$+ J^{-2/3}\left(\hat{\mathbf{T}}_r - \tfrac{1}{3}\left(\hat{\mathbf{T}}_r : \hat{\mathbf{C}}\right)\hat{\mathbf{C}}^{-1}\right) + \mu_e J^{-2/3}\left(\hat{\mathbf{C}}_{\mathbf{i}}^{-1} - \tfrac{1}{3} tr\left(\hat{\mathbf{C}}_{\mathbf{i}}^{-1}\hat{\mathbf{C}}\right)\hat{\mathbf{C}}^{-1}\right)$$

- Evolution equations

$$\dot{\hat{\mathbf{T}}}_r = q_r(t)\,\overset{4}{\mathbf{C}}(t) : \dot{\hat{\mathbf{C}}}$$

→ Evolution eq. for the stress of the newly reformed network

$$\dot{\hat{\mathbf{C}}}_{\mathbf{i}}{}^{j} = 2\left(\mathbf{C} - \tfrac{1}{3} tr\left(\mathbf{C}\left(\hat{\mathbf{C}}_{\mathbf{i}}{}^{j}\right)^{-1}\right)\hat{\mathbf{C}}_{\mathbf{i}}{}^{j}\right) \Big/ \tau^{j}(\theta)$$

→ Evolution eq. for inelastic deformation

$$\dot{q}_d = \frac{1}{j}\sum_j c\,\nu_d^j \exp\left(\frac{-E_d^j}{R\theta}\right)\left(1 - q_d^j\right)$$

$$\dot{q}_r = \frac{1}{j}\sum_j c\,\nu_r^j \exp\left(\frac{-E_r^j}{R\theta}\right)\left(1 - q_r^j\right)$$

→ Evolution eq. for the internal (aging) variables *qd* and *qr*

Johlitz (2012)

Modelling

Set of constitutive eq. and evolution eq. can be evaluated

- Heat flux, diffusion flux, reaction term

$$\mathbf{q} = -\lambda_\theta \,\mathrm{Grad}\theta - \lambda_c\left(\varsigma\,\delta^2 + \varsigma\,\delta\,\theta\right) c\,\mathrm{Grad}c$$

$$\mathbf{j} = -\lambda_c\left(\delta + \varsigma\,\theta\right)\mathrm{Grad}c$$

$$\hat{c} = -k\left(\delta\, c + \varsigma\, c\,\theta\right)$$

Johlitz (2012)

$\delta = 1 \quad \varsigma = 0$ →

$$\mathbf{q} = -\lambda_\theta \,\mathrm{grad}\theta \quad \text{(Fourier's law)}$$

$$\mathbf{j} = -\lambda_c \,\mathrm{grad}c \quad \text{(Fick's law)}$$

$$\hat{c} = -k\, c \quad \text{(linear reaction)}$$

- Temperature and aging dependency of diffusion and reaction coefficient Johlitz (2012)

$$\lambda_c = \lambda_{c_0} \exp\left(-\frac{E_c}{R\theta}\right) \exp\left(-\gamma\, q_r\right)$$

$$k = \left[k_{01}\left(1 - q_d\right) + k_{02}\left(1 - q_r\right)\right] \exp\left(-\frac{E_k}{R\theta}\right)$$

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Implementation

Weak formulation of the problem

$$0 = \int_{\Omega} \text{weak}\ \partial V$$

- Balance momentum equation

$$0 = -\int_V \delta \boldsymbol{E}(\boldsymbol{u}) : \widetilde{\boldsymbol{T}}(\theta, c, q_d(c), q_r(c))\, dV - \int_V \delta \boldsymbol{u}\, \boldsymbol{b}\, dV + \int_S \delta \boldsymbol{u}\, \boldsymbol{t}\, dS$$

- Heat conduction equation

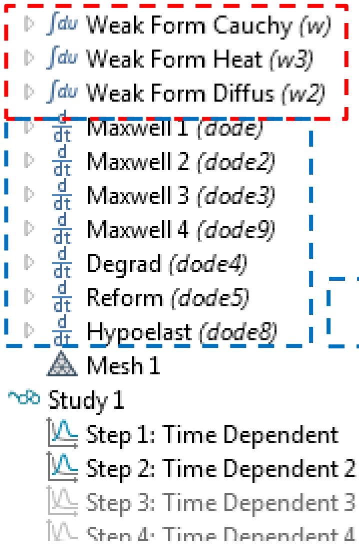
$$0 = -\int_V \delta\theta\, \rho\, c_p\, \dot{\theta}\, dV - \int_V Grad(\delta\theta)\, [\lambda_\theta Grad\theta + \lambda_c[\zeta\delta^2 + \zeta\delta\theta]\, c\, Grad c] dV - \int_S \delta\theta\, q^* dS$$

- Diffusion-Reaction equation

$$0 = -\int_V \delta c[\rho\dot{c} + k[c\,\delta + \zeta c\,\theta]] dV - \int_V Grad(\delta c)\, \lambda_c(\delta + \zeta\,\theta) Grad c\, dV - \int_S \delta c\, j^* dS$$

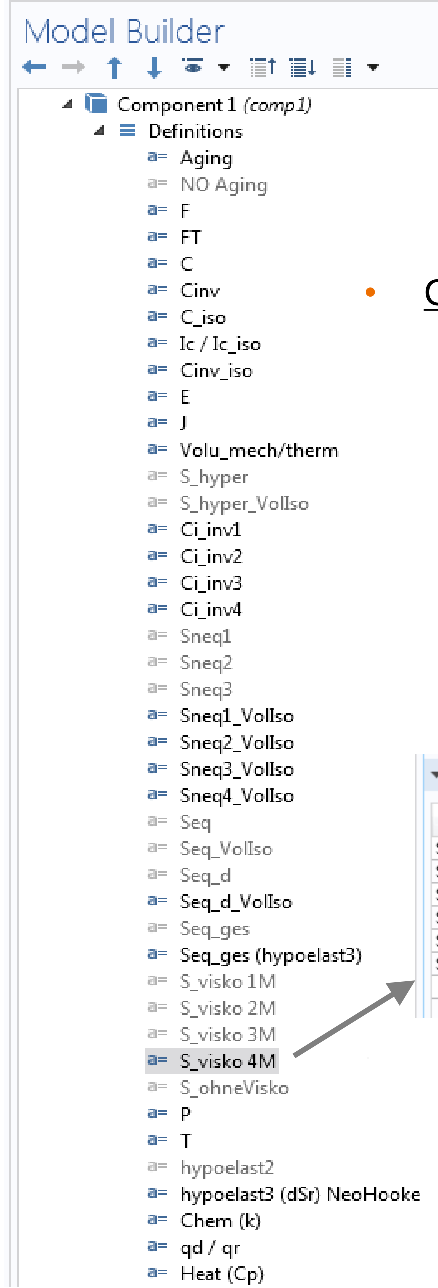
→ Strongly coupled multifield problem

Implementation

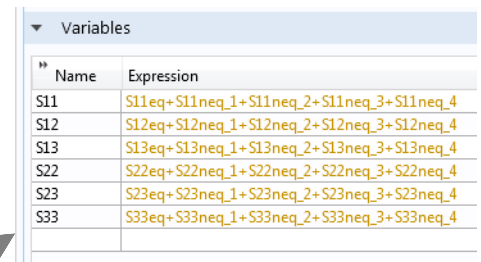


Weak form eq.

Evolution eq.



- Created tensor library:
  - Basic tensors
  - Constitutive laws
  - Auxiliary variables



Name	Expression
S11	S11eq+S11neq_1+S11neq_2+S11neq_3+S11neq_4
S12	S12eq+S12neq_1+S12neq_2+S12neq_3+S12neq_4
S13	S13eq+S13neq_1+S13neq_2+S13neq_3+S13neq_4
S22	S22eq+S22neq_1+S22neq_2+S22neq_3+S22neq_4
S23	S23eq+S23neq_1+S23neq_2+S23neq_3+S23neq_4
S33	S33eq+S33neq_1+S33neq_2+S33neq_3+S33neq_4

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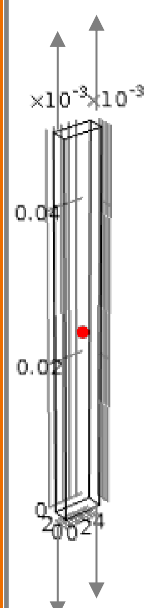
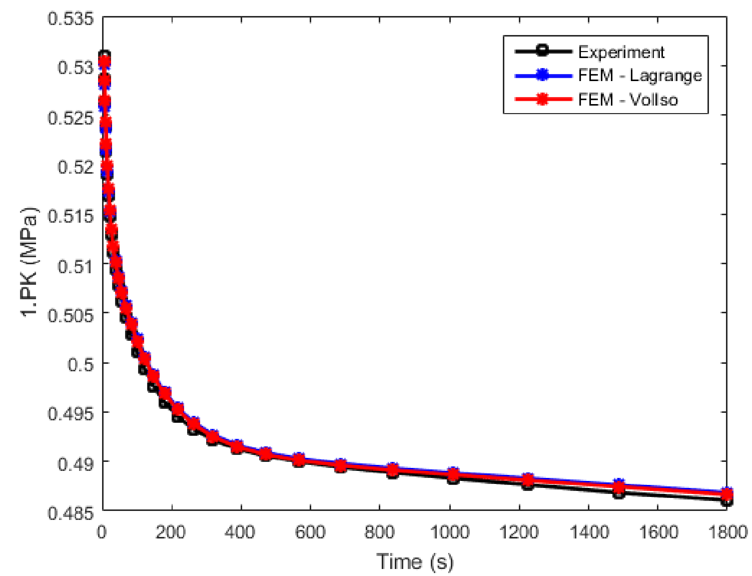
Simulations

- Measured parameters
  - Material parameters: $\mu_0, \mu_r, \mu_e, \tau(\theta)$
  - Aging parameters: E_d, ν_d, E_r, ν_r
  - Thermal parameters: $c_p(\theta), \alpha(\theta), \lambda_\theta$

- Estimated parameters
  - Chemical parameters: $\lambda_{c_0}, E_c, k_{01}, k_{02}, E_k, \gamma, \delta, \varsigma$

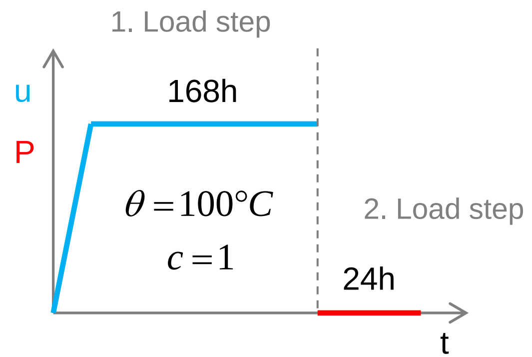


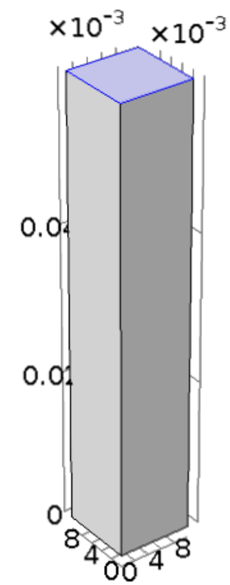
- 3D uniaxial relaxation test in tension
- Model without aging
- **Comsol vs. Experiment** (NBR rubber)



Simulations

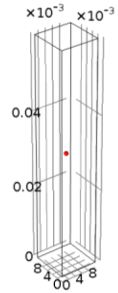
- BC:
  - 1. LS – applied displacement u
  - 2. LS – applied zero stress P

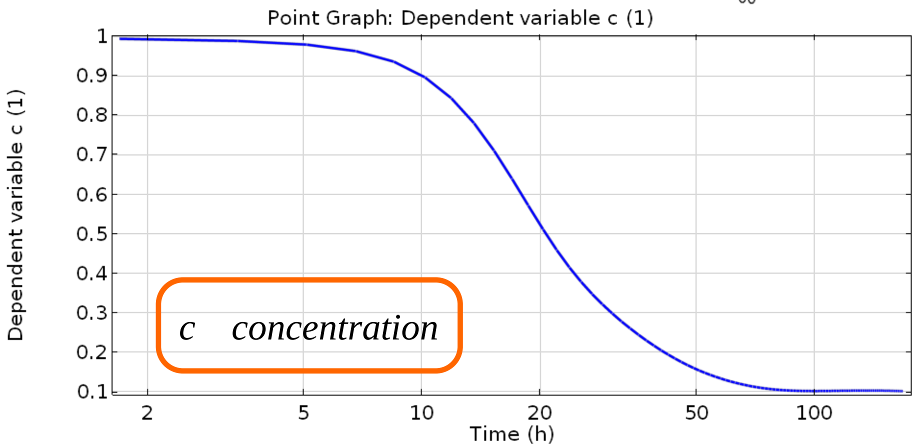


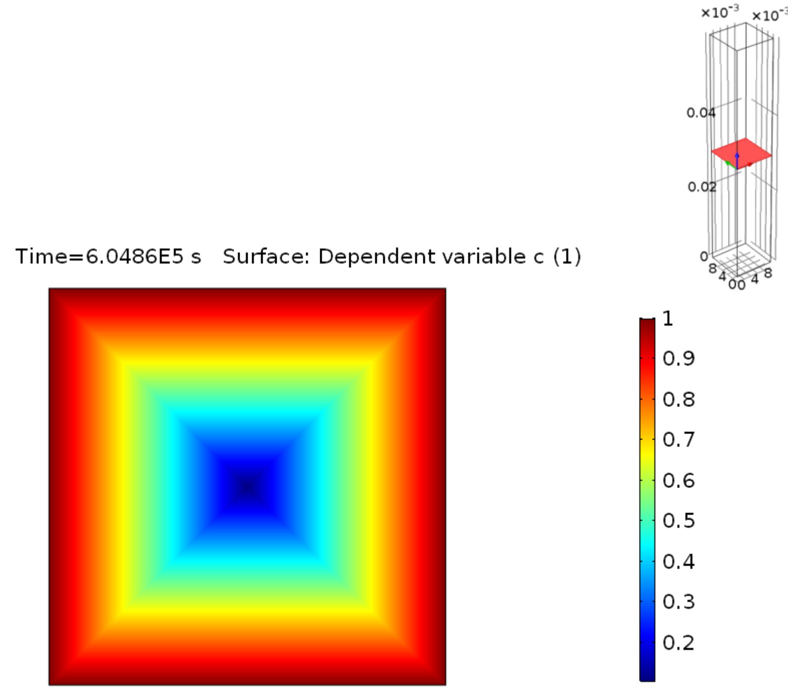


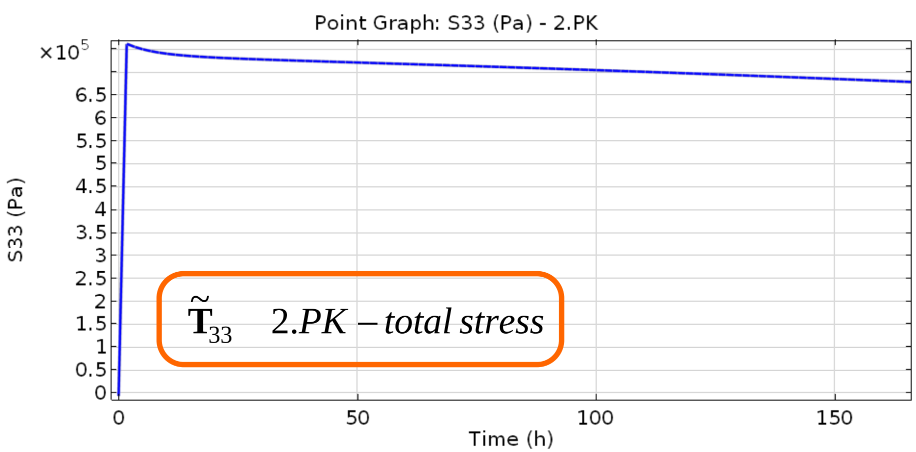
Simulations

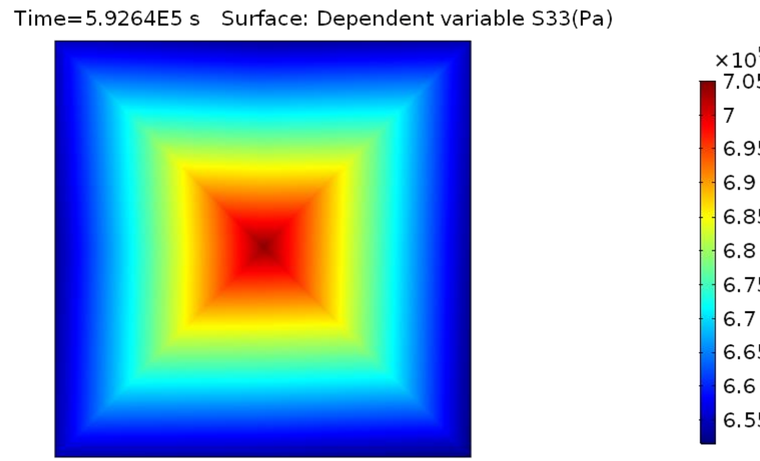
- 1. Load step results





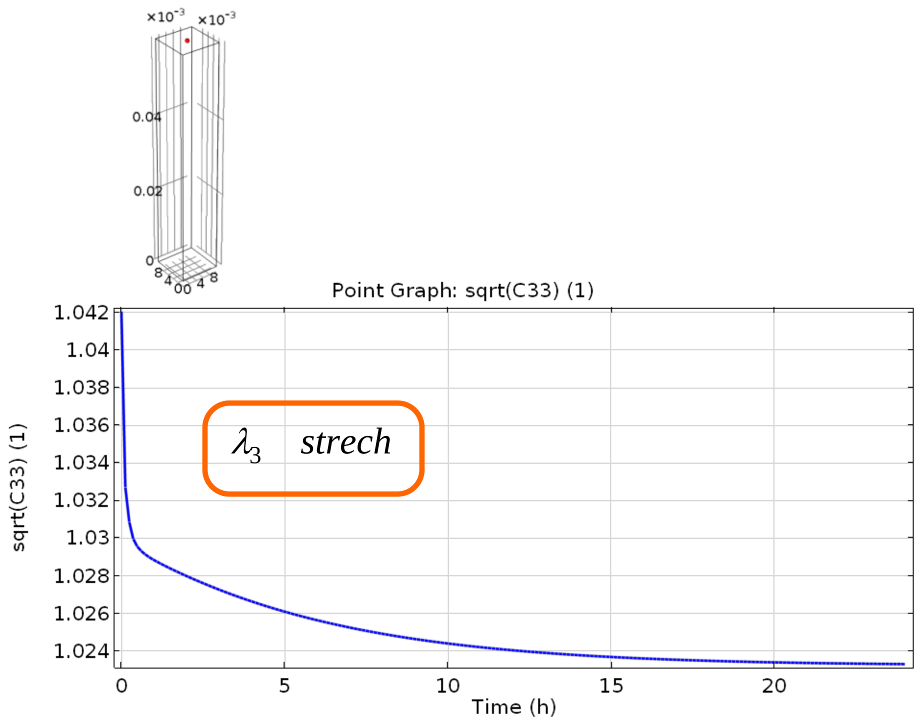


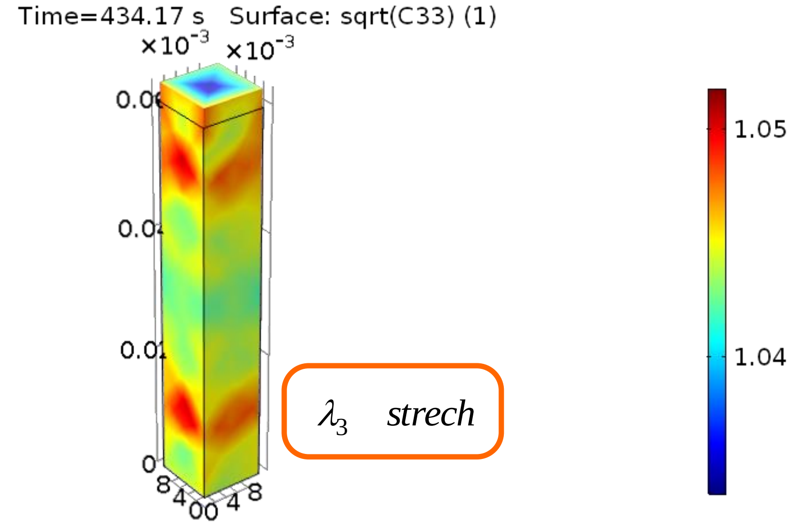


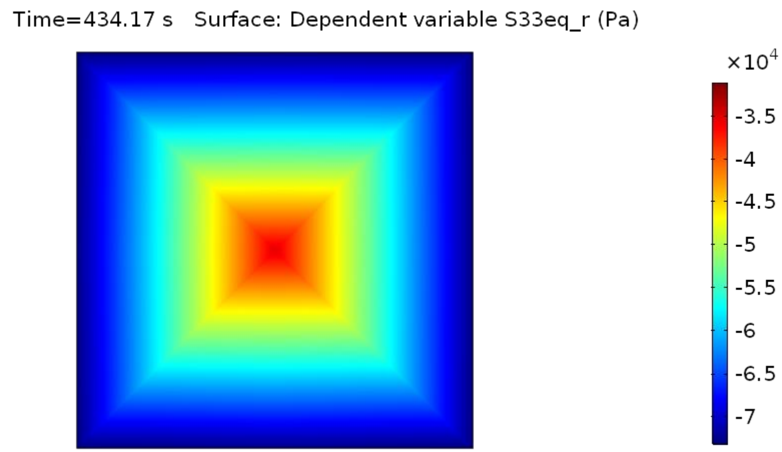


Simulations

- 2. Load step results







$\tilde{\mathbf{T}}_{r_{33}}$ 2.PK – Stress of reformated network

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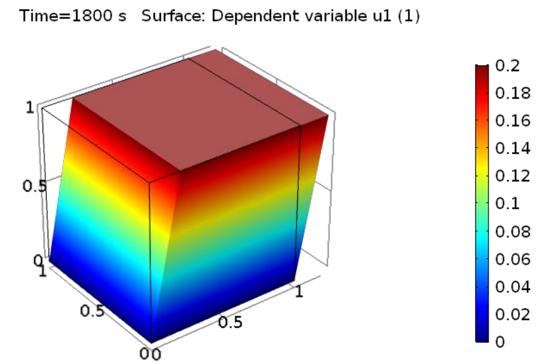
Summary & outlook

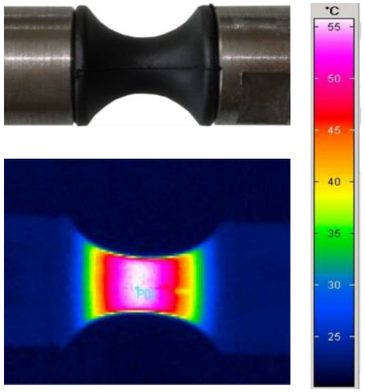


Summary

- Introduction to aging processes
- Model overview – phenomenological approach
- Modeling of aging, tension set and DLO effect
- Modeling of material behavior: nonlinear thermoviscoelasticity

Outlook

- Experimental identification of chemical parameters
- Simulation of an industrial component
- Include aging due to dissipative heating



Thank you.