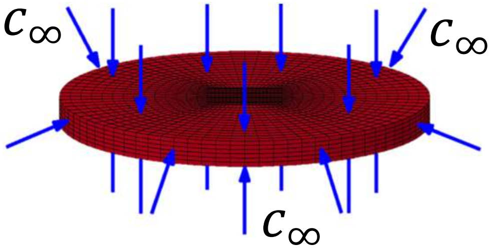
16. LS-DYNA Forum 2022

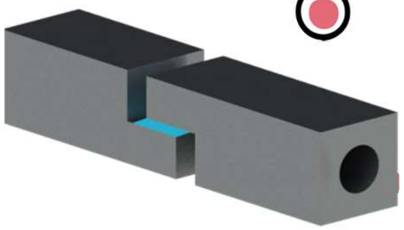
October 11 - 12, 2022, Bamberg, Germany

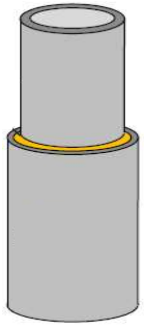
Fabian Kötz, Anton Matzenmiller

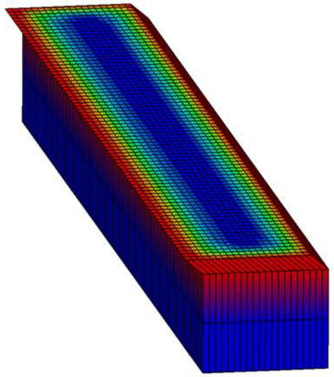
Method Development: Characterization, Modeling and Simulation of Hygro-Thermo Effects in Thick Layer Adhesives

Institute of Mechanics – Department of Mechanical Engineering – University of Kassel, Germany





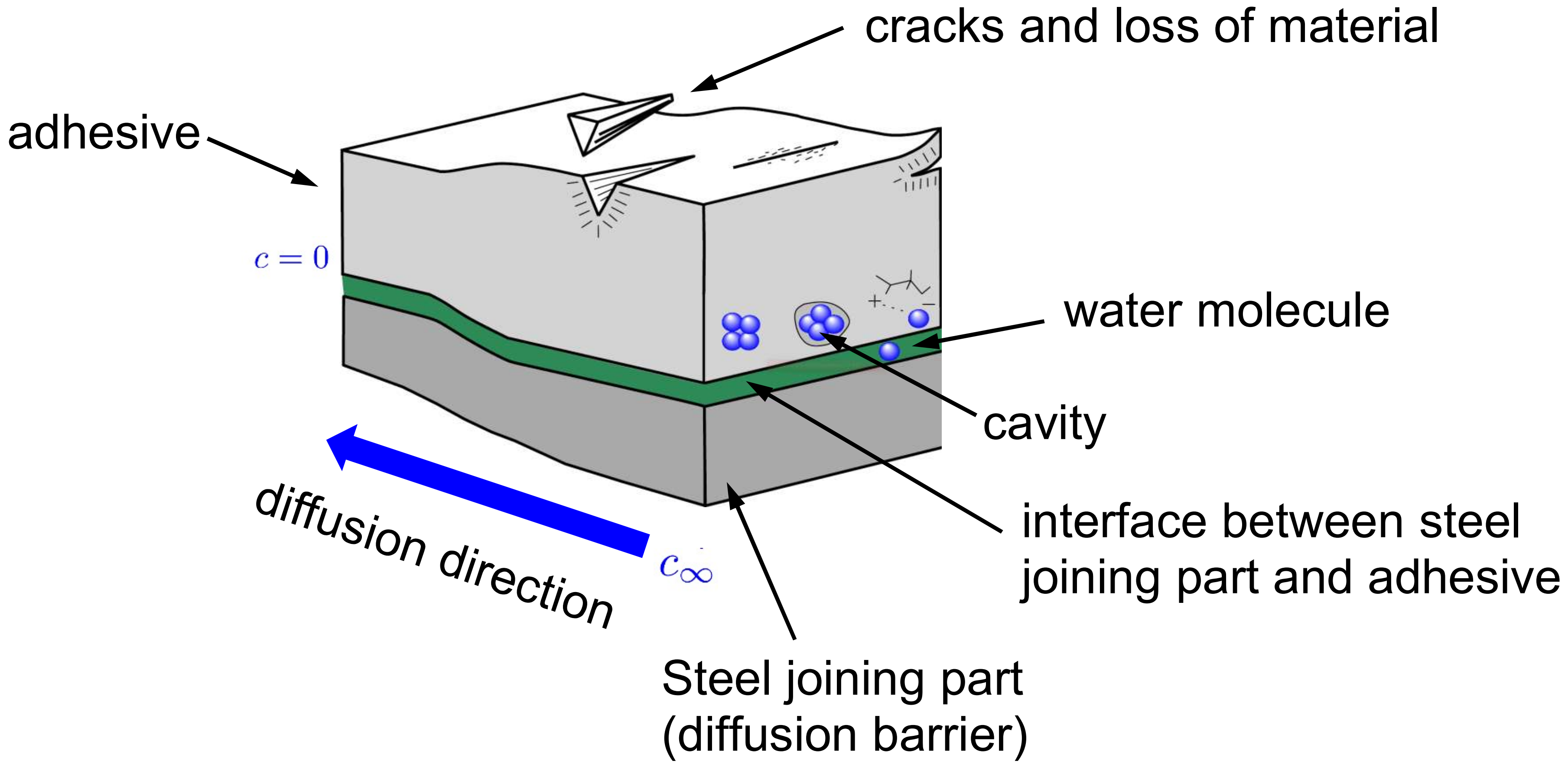




Agenda

- Motivation
- Moisture simulation with LS-DYNA
- Material model for the adhesive
    - Reversible effects
    - Irreversible damage
- Simulation and validation

Effects: Water diffusion in adhesive



cracks and loss of material

adhesive

$c = 0$

water molecule

cavity

interface between steel
joining part and adhesive

diffusion direction

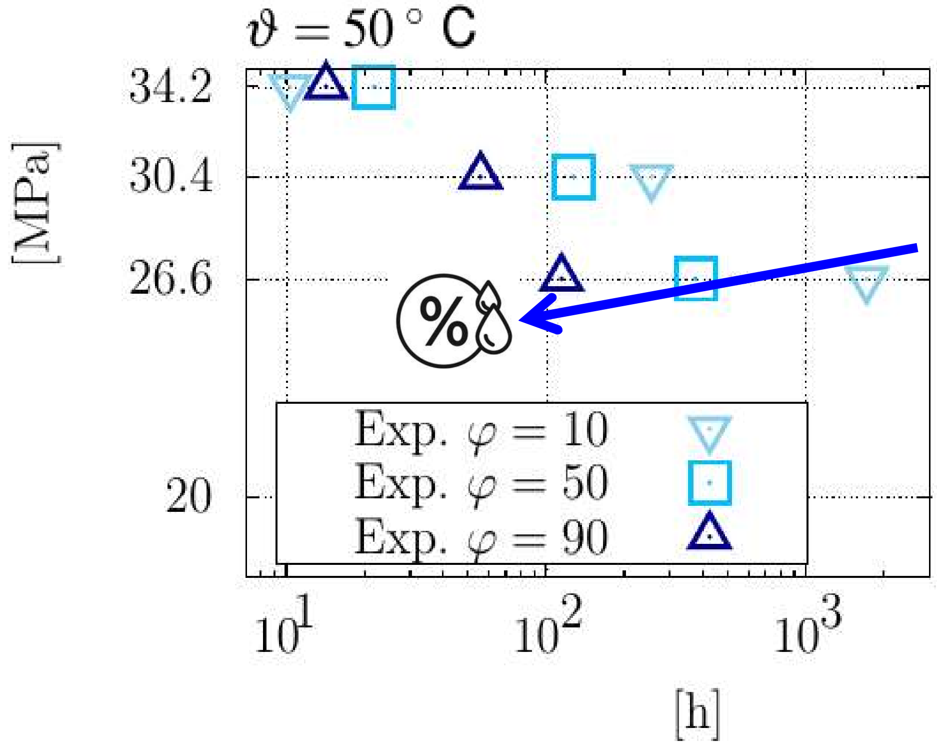
c_∞

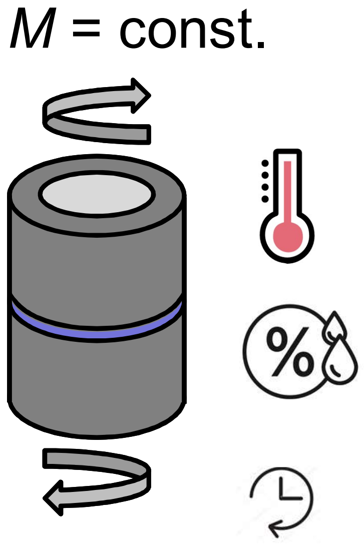
Steel joining part
(diffusion barrier)

[1] D. A. Bond, P. A. S. (2006). Applied Mechanics Reviews, 59(1-6):249 – 268.

Motivation

Successive degradation of stiffness and strength due to damage resulting from chemical aging





→ Significant reduction of lifetime: depending on humidity, temperature and loading

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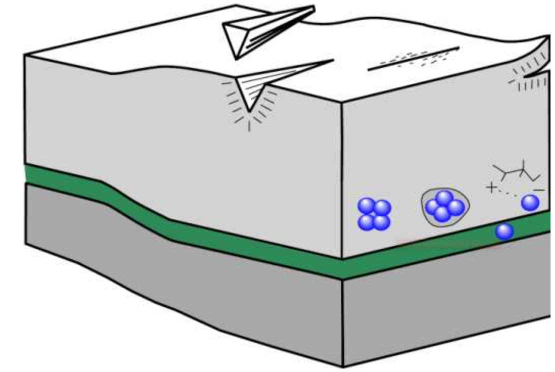
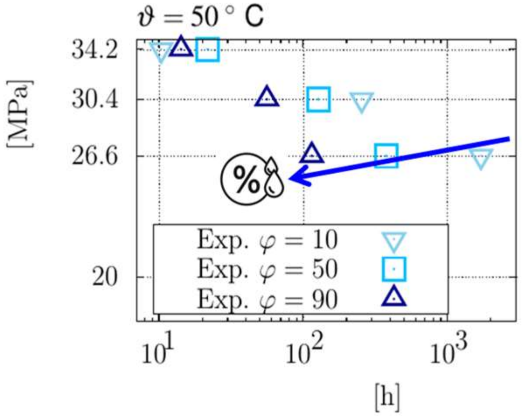
[1] Bieker, C. (2006). “Methodenentwicklung zur Bestimmung des hygrothermo-mechanischen Langzeitverhaltens von strukturellen Klebverbindungen mit metallischen und mineralischen Untergründen”. Schriftenreihe des Instituts für Werkstofftechnik Kassel. Shaker. Dissertation.

Procedure for determining the diffusion properties

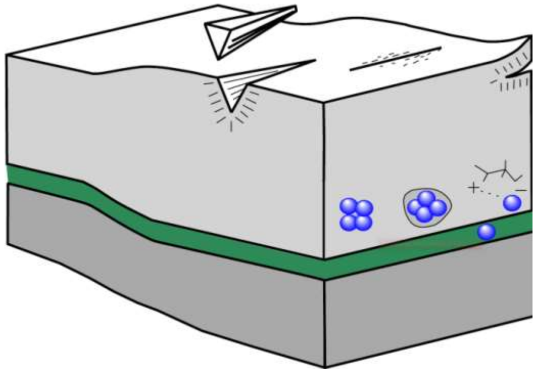


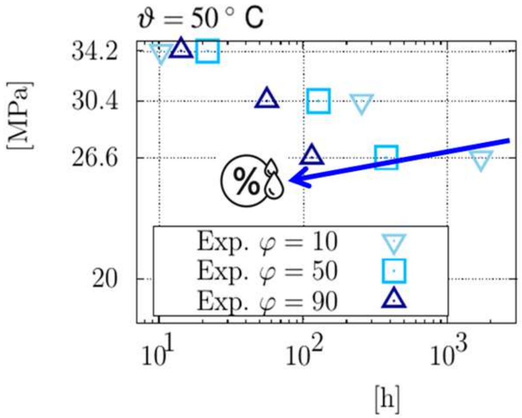


Model development, which describes the **hygro-thermo-mechanical** influences on the service life of the adhesive layer

First step: Description of the diffusion behavior
Second step: Classification into reversible and irreversible damage by water
Third step: Combination with the material model and thermo-mechanical damage

Procedure for determining the diffusion properties



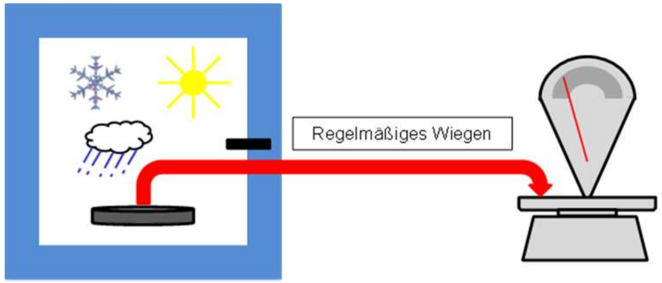


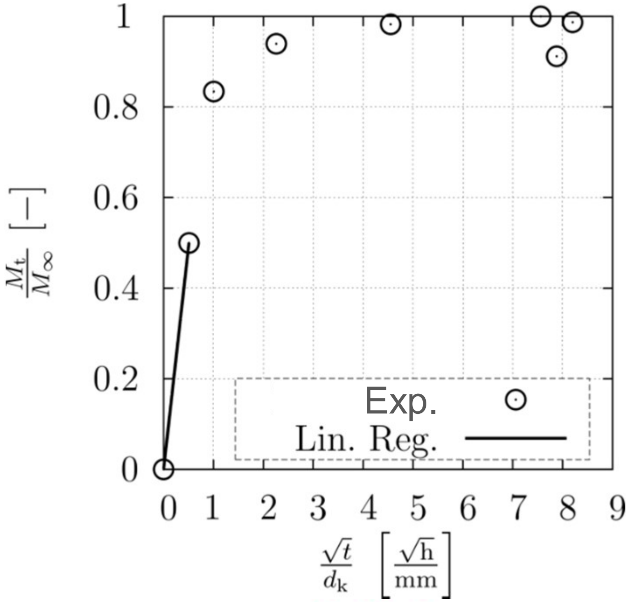
Model development, which describes the **hygro-thermo-mechanical** influences on the service life of the adhesive layer

First step: **Description of the diffusion behaviour**

Modeling moisture absorption

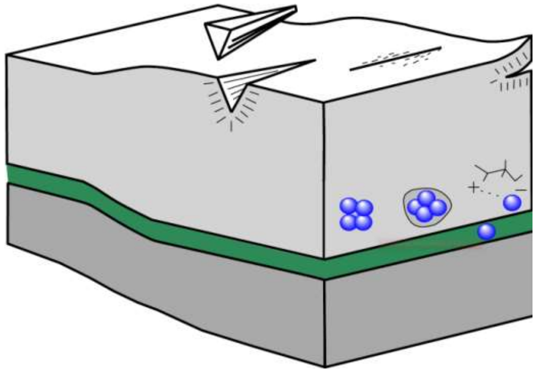
Experimental investigation based on adhesive samples

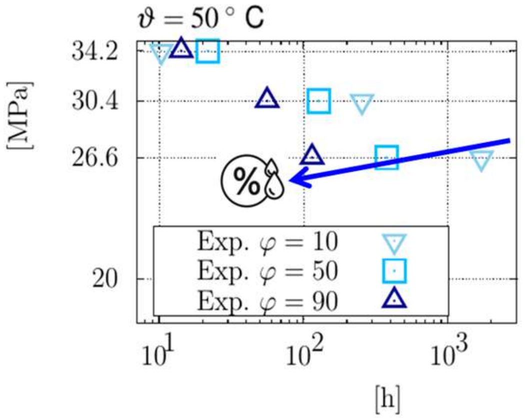




[1] Laboratorium für Werkstoff und Fügetechnik, Paderborn, Prof. Meschut

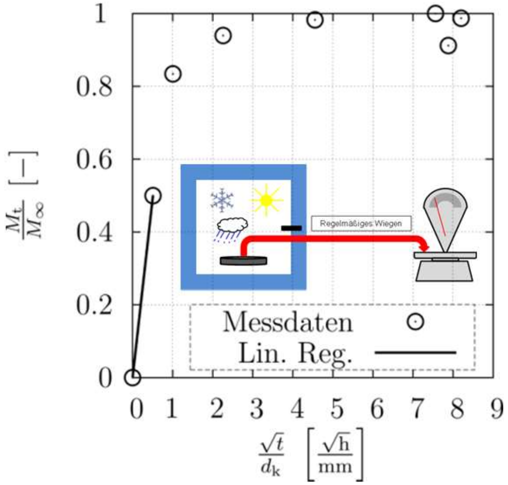
Procedure for determining the diffusion properties





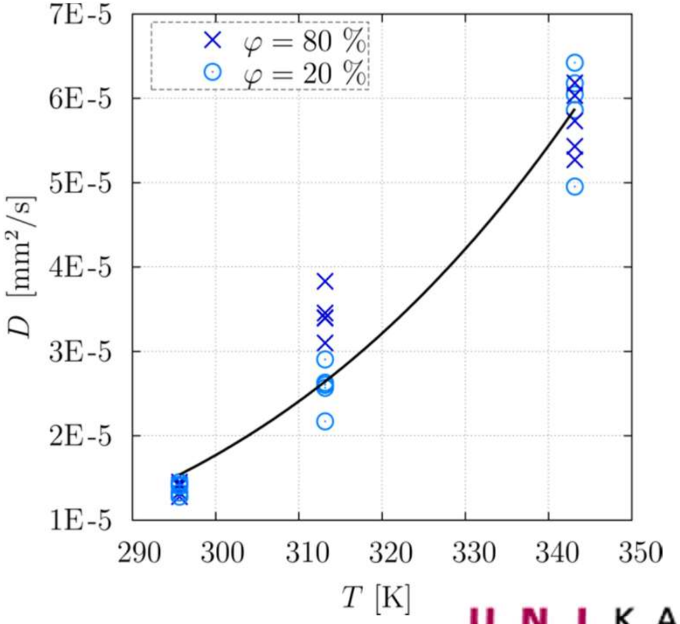
Model development, which describes the **hygro-thermo-mechanical** influences on the service life of the adhesive layer

First step: **Description of the diffusion behaviour**



Diffusion coefficient:

$$D = D_0 \exp\left(D_1\left(\frac{1}{T_{\mathrm{ref}}} - \frac{1}{T}\right)\right)$$

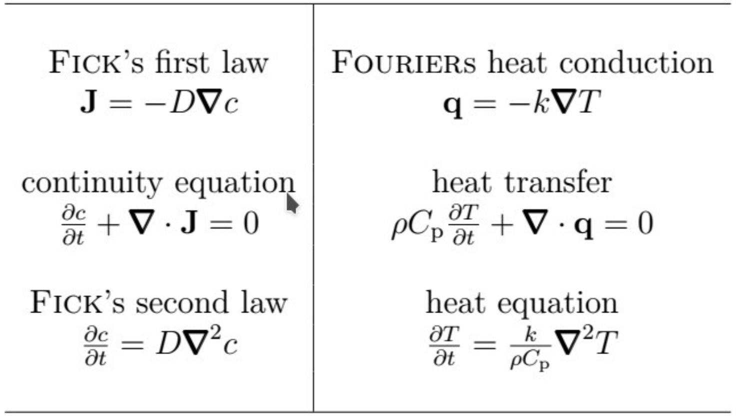


[1] Crank, The Mathematics of Diffusion, 1975
[2] Laboratorium für Werkstoff und Fügetechnik, Paderborn, Prof. Meschut
[3] Abdel-Wahab et al., Diffusion of Moisture in Adhesively Bonded Joints, 2001

Moisture Simulation with LS-DYNA

LS-DYNA has no diffusion solver, therefore the temperature solver is used

Diffusion Thermal conduction



Diffusion	Thermal conduction
FICK's first law $\mathbf{J} = -D\boldsymbol{\nabla}c$	FOURIERs heat conduction $\mathbf{q} = -k\boldsymbol{\nabla}T$
continuity equation $\frac{\partial c}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{J} = 0$	heat transfer $\rho C_{\mathrm{p}}\frac{\partial T}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{q} = 0$
FICK's second law $\frac{\partial c}{\partial t} = D\boldsymbol{\nabla}^2 c$	heat equation $\frac{\partial T}{\partial t} = \frac{k}{\rho C_{\mathrm{p}}}\boldsymbol{\nabla}^2 T$

Moisture Simulation with LS-DYNA

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concentration c	temperature T
mass flow $\mathbf{J}$	heat flow $\mathbf{q}$
diffusion coefficient D	thermal conductivity k
1	specific heat capacity C_p
1	density ρ

The `*THERMAL_SOLVER` of LS-DYNA can be used for the solution of the hygric field problem,

the diffusion and thermal problems have analogous field equations and boundary conditions

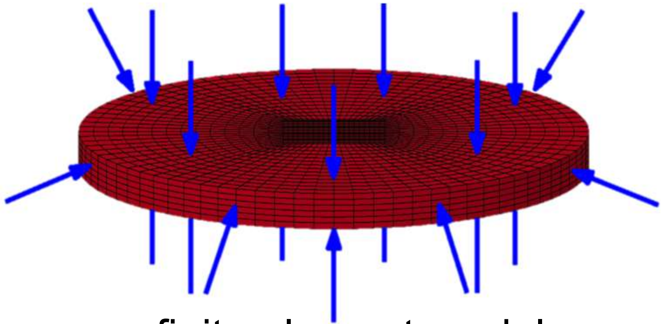
Moisture Simulation with LS-DYNA

LS-DYNA has no diffusion solver, therefore the temperature solver is used

Diffusion	Thermal conduction
Fick's first law $\mathbf{J} = -D\boldsymbol{\nabla} c$	Fouriers heat conduction $\mathbf{q} = -k\boldsymbol{\nabla} T$
continuity equation $\frac{\partial c}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{J} = 0$	heat transfer $\cancel{\rho C_\mathrm{p}} \frac{\partial T}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{q} = 0$
Fick's second law $\frac{\partial c}{\partial t} = D\boldsymbol{\nabla}^2 c$	heat equation $\frac{\partial T}{\partial t} = \frac{k}{\cancel{\rho C_\mathrm{p}}}\boldsymbol{\nabla}^2 T$

concentration c	temperature T
mass flow $\mathbf{J}$	heat flow $\mathbf{q}$
diffusion coefficient D	thermal conductivity k
$\boxed{1}$	specific heat capacity C_p
$\boxed{1}$	density ρ

adhesive sample



finite element model

***BOUNDARY_TEMPERATURE_SET**

***MAT_THERMAL_ISOTROPIC**

Moisture Simulation with LS-DYNA

LS-DYNA has no diffusion solver, therefore the temperature solver is used

Diffusion	Thermal conduction
FICK's first law $\mathbf{J} = -D\boldsymbol{\nabla}c$	FOURIERs heat conduction $\mathbf{q} = -k\boldsymbol{\nabla}T$
continuity equation $\frac{\partial c}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{J} = 0$	heat transfer $\cancel{\rho C_\mathrm{p}}\frac{\partial T}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{q} = 0$
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concentration c	temperature T
mass flow $\mathbf{J}$	heat flow $\mathbf{q}$
diffusion coefficient D	thermal conductivity k
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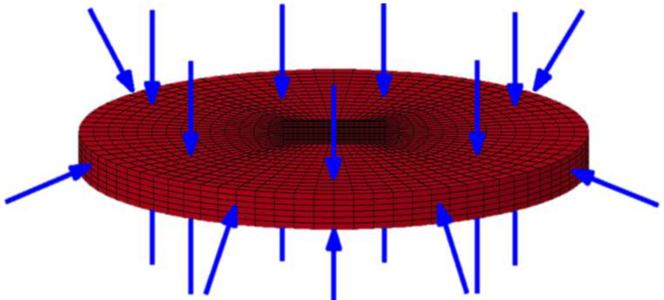
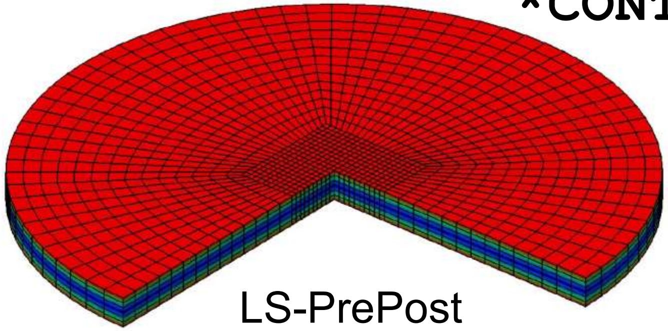
adhesive sample

→



finite element model

```
*BOUNDARY_TEMPERATURE_SET
*MAT_THERMAL_ISOTROPIC
*CONTROL_THERMAL_SOLVER
```



LS-PrePost

temperature → concentration

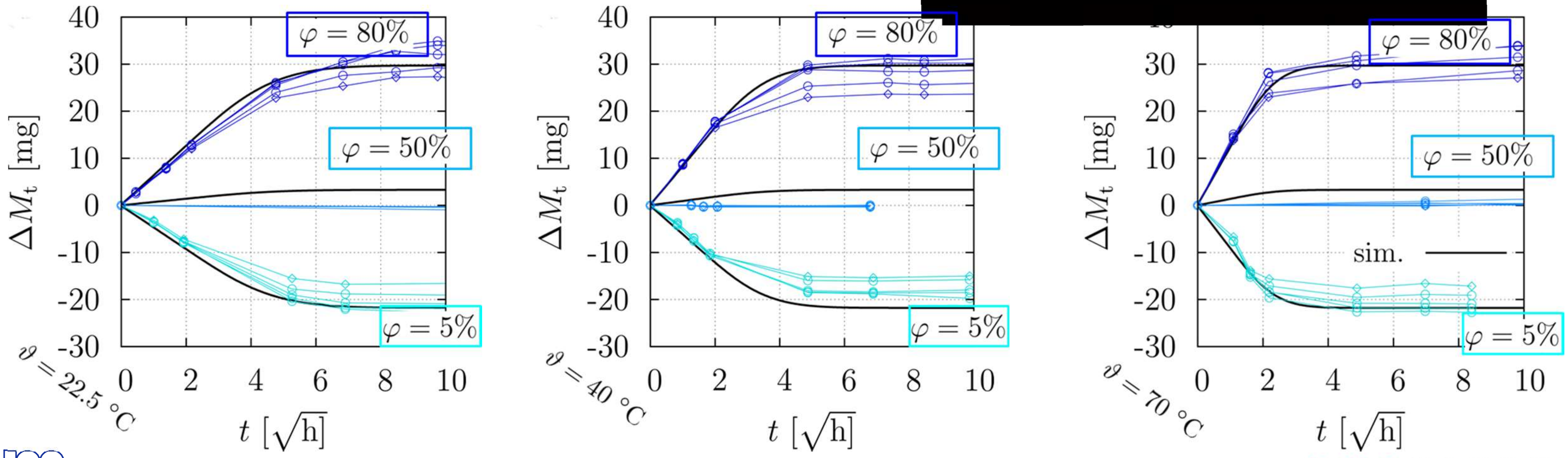
Moisture Simulation with LS-DYNA

Verification of the parameter identification

$$M = \underbrace{A \cdot d_{\mathrm{k}}}_{V} \cdot c \quad \longleftrightarrow T$$

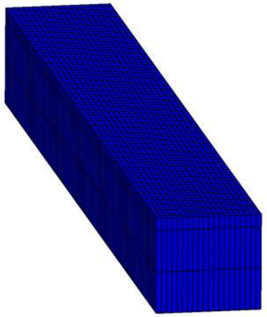
[redacted]

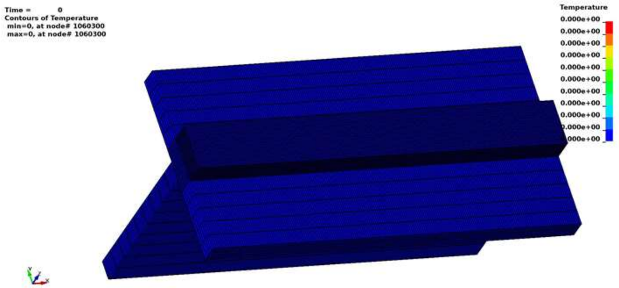
Comparison of experiment and calculation: good agreeme



Concentration calculation in different adhesive bonding specimens

Successful simulation of water absorption is used to calculate the concentration in any sample geometries





butt joint specimen shear specimen component-like specimen

Concentration used as damage driving variable for calculation of reversible effects and irreversible damage

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Description of the semi-structural adhesive behaviour under aging

Thermal component

Presetting the temperature

T

Hygric component

Fick's model

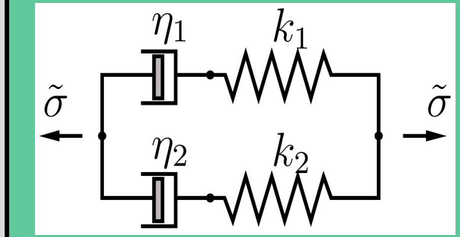
$$\frac{\partial c}{\partial t} = D \nabla^2 c$$

Diffusion model

Mechanical component:

Finite viscoelasticity

Linear viscoelasticity



Rheological model

Hyperelasticity

Mooney-Rivlin model
Simo model
Ogden model

→ non-linear behaviour
→ thick adhesive layers
→ large deformations

Continuum damage mechanics

$$\sigma = (1 - D_{\mathrm{ca}})\tilde{\sigma} \qquad \dot{D}_{\mathrm{ca}} = \dot{D}_{\mathrm{ca}}(D_{\mathrm{ca}}, \sigma, c, T)$$

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Reversible effects: Time-concentration-temperature shift

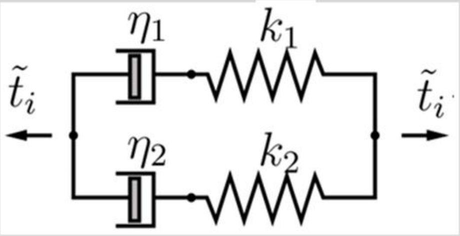
Adhesive layer model

Damage model

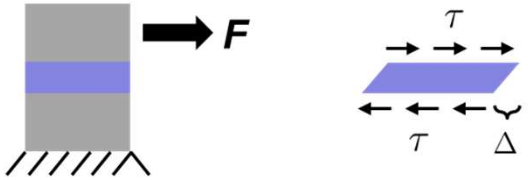
Irreversible effects

$$\dot{D}_{\text{ca}} = \dot{D}_{\text{ca}}(D, \sigma_{\text{eqc}}(t_i), c, T)$$

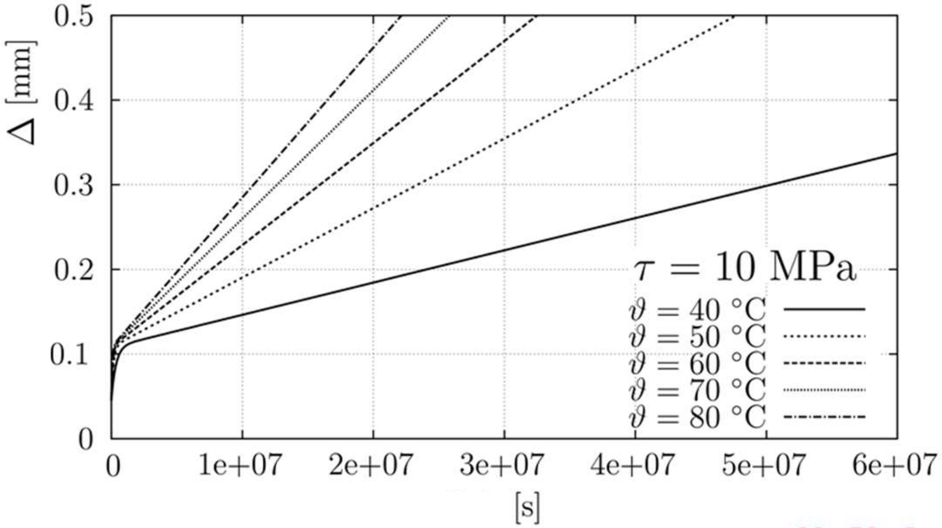
Rheological model



Reversible effects

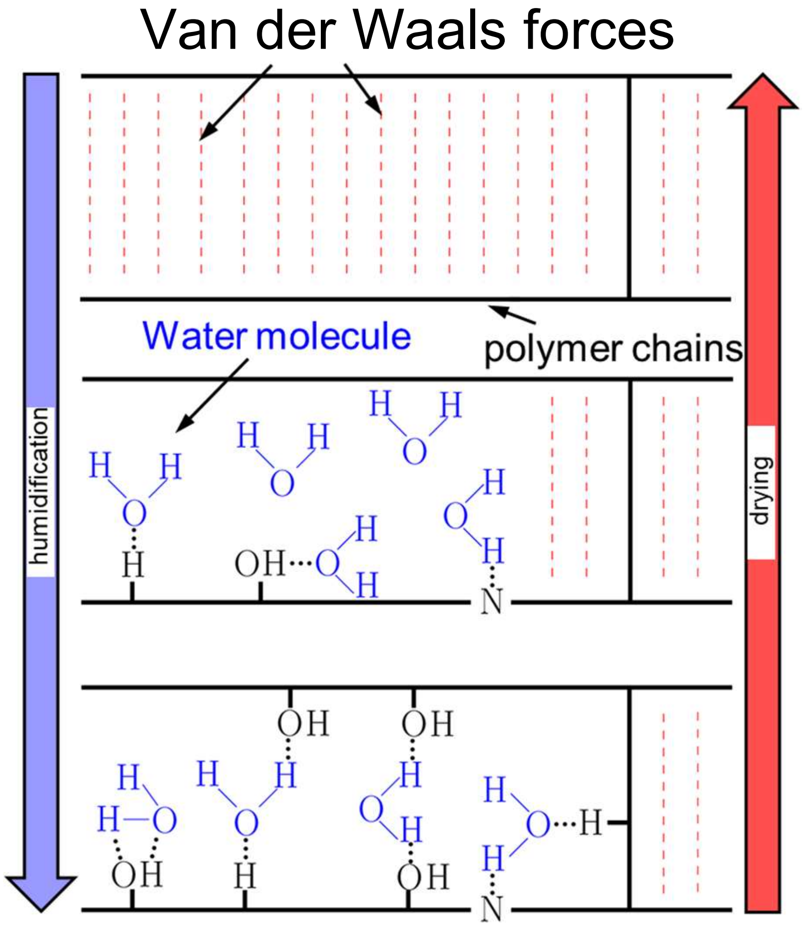


Faster creep / relaxation
at higher temperatures



Concentration as reversible damaging factor

Reversible effect



- Water diffuses between polymer chains when moistened and breaks down Van der Waals forces
- Hydrogen bonds can be dissolved again by drying (higher temperature may be necessary).
- Water diffuses out completely during drying
- (thermo-)reversible in the chemical sense [2].

[1] Zhou, J. and Lucas, J. P. (1999). Polymer, 40(20):5505–5512.
[2] Petrie, E. (2005). Epoxy Adhesive Formulations, S. 319

Reversible effects: Time-concentration-temperature shift

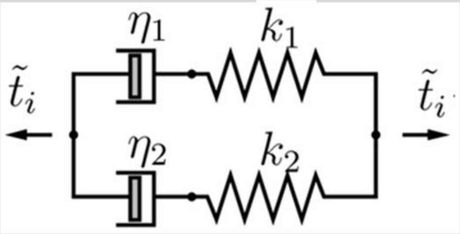
Adhesive layer model

Damage model

Irreversible effects

$$\dot{D}_{\mathrm{ca}} = \dot{D}_{\mathrm{ca}}(D, \sigma_{\mathrm{eqc}}(t_i), c, T)$$

Rheological model



Reversible effects

Modeling of the reversible effect of temperature and concentration

WIECHERT-/ MAXWELL-Model: $$R(t-\tau, T) = k_\infty + \sum_{i=1}^{M} k_i \exp\left(-\frac{t-\tau}{a_{\mathrm{T}}(T)\hat{\tau}_i}\right)$$

Time-temperature-shift: $a_{\mathrm{T}}(T)$

Time-concentration-temperature shift: $a_{\mathrm{res}}(T, c) = a_{\mathrm{T}}(T) a_{\mathrm{c}}(c)$

Reversible effects: Time-concentration-temperature shift

Time-concentration-temperature shift: $a_{\mathrm{res}}(T,c) = a_{\mathrm{T}}(T)a_{\mathrm{c}}(c)$

Approach for time-temperature shift function

$$\log a_{\mathrm{T}}(T) = \frac{-p_{\mathrm{T1}}(T - T_{\mathrm{aT}})}{p_{\mathrm{T2}} + T - T_{\mathrm{aT}}}$$

WILLIAMS-LANDEL-FERRY-(WLF-) [1,2]

$$\log a_{\mathrm{T}}(T) = E_{\mathrm{A}}\left(\frac{1}{T} - \frac{1}{T_{\mathrm{aT}}}\right)$$

ARRHENIUS [2]

Transfer to time concentration shift function

$$\log a_{\mathrm{c}}(c) \overset{[3,4]}{=} \frac{-p_{\mathrm{c1}}(c - c_{\mathrm{ac}})}{p_{\mathrm{c2}} + c - c_{\mathrm{ac}}}$$

$$\ln a_{\mathrm{c}}(c) \overset{[5]}{=} p_{\mathrm{c1}} + p_{\mathrm{c2}}\left(1 - \exp\left(\frac{c_{\mathrm{ac}} - c}{p_{\mathrm{c3}}}\right)\right)$$

***usermat**

[1] Williams et. Al., 1955 [2] s. FOSTA-Projekt P 1087 [3] Maksimov et. al, 1972 [4] Ma et. al, 2006 [5] Zheng et. al, 2004

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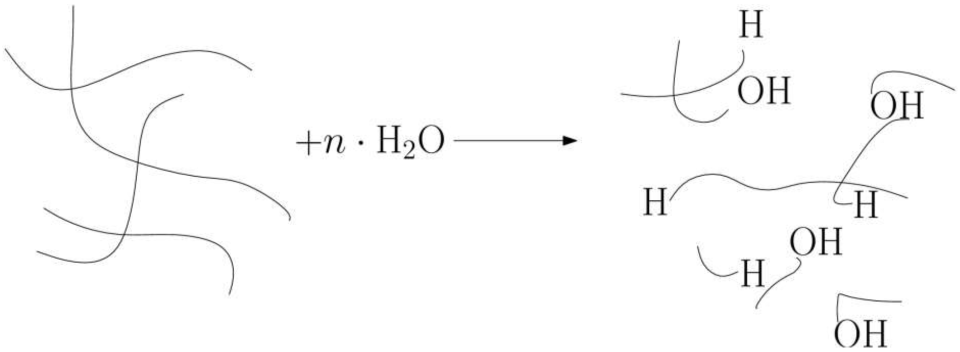
    - Irreversible damage

- Simulation and validation

Concentration as irreversible damaging factor

Irreversible effects [2,3]



- Breaking of the polymer chains by hydrolysis
- Previously intact chemical bonds in the polymer cannot be restored by drying
- irreversible in the chemical meaning
- Stress reduces activation energy for hydrolysis

[1] Zhou, J. and Lucas, J. P. (1999). Polymer, 40(20):5505–5512.
[2] Petrie, E. (2005). Epoxy Adhesive Formulations, S. 319
[3] Comyn, J. (1997). Adhesion Science, S. 133

Damage model – Differential equation

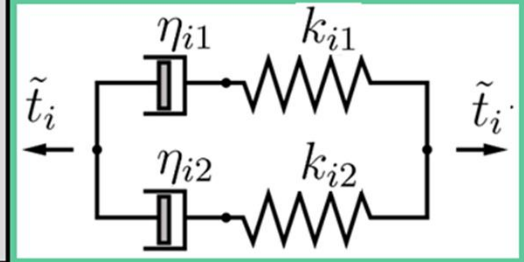
Adhesive layer model

Damage model

Irreversible effects

$$\boxed{\dot{D}_{\mathrm{ca}} = \dot{D}_{\mathrm{ca}}(D, \sigma_{\mathrm{eqc}}(t_i), c, T)}$$

Rheological model



Reversible effects

$$\dot{D}_{\mathrm{ca}} = \underbrace{\frac{1}{c_0}\left(\frac{\sigma_{\mathrm{eqc}}}{\sigma_{\mathrm{ref}}(1-D_{\mathrm{ca}})}\right)^{n} \exp\left(p_{\mathrm{c}}\left(\frac{1}{T_{\mathrm{refc}}}-\frac{1}{T}\right)\right)}_{\dot{D}_{\mathrm{c}}} + \underbrace{B_{\mathrm{a}}(1-D_{\mathrm{ca}})\left(\frac{c}{c_{\infty,\mathrm{ref}}}\right)^{l} \exp\left(p_{\mathrm{a}}\left(\frac{1}{T_{\mathrm{refa}}}-\frac{1}{T}\right)\right)}_{\dot{D}_{\mathrm{a}}}$$

$c_0 = 1\ \mathrm{s}$

Creep damage

Aging damage / hygro damage

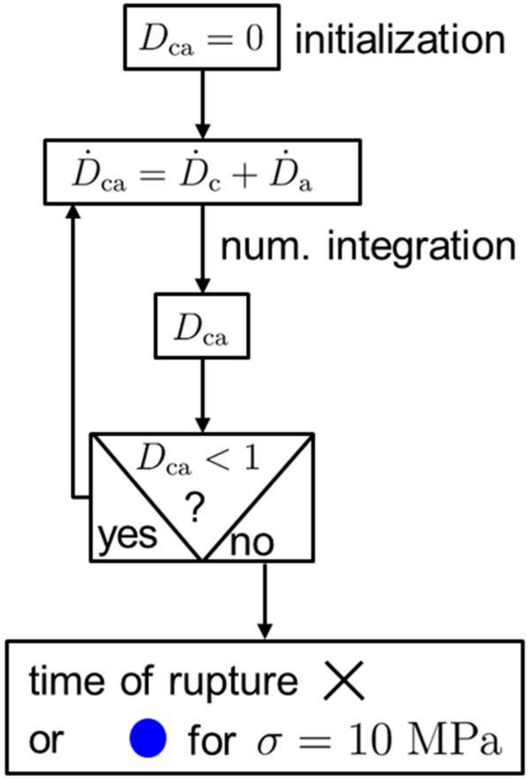
Parameter: $\sigma_{\mathrm{ref}}\,,\, n\,,\, T_{\mathrm{refc}}\,,\, p_{\mathrm{c}}$ $\quad B_{\mathrm{a}}\,,\, l\ ,\, T_{\mathrm{refa}}\,,\, p_{\mathrm{a}}$

Solution with LS-DYNA: Hygro-thermo-mechanical damage

$$\dot{D}_{\mathrm{ca}} = \underbrace{\frac{1}{c_0}\left(\frac{\sigma}{\sigma_{\mathrm{ref}}(1-D_{\mathrm{ca}})}\right)^{n} \exp\left(p_{\mathrm{c}}\left(\frac{1}{T_{\mathrm{refc}}}-\frac{1}{T}\right)\right)}_{\dot{D}_{\mathrm{c}}} + \underbrace{B_{\mathrm{a}}(1-D_{\mathrm{ca}})\frac{c}{c_{\infty,\mathrm{ref}}}\exp\left(p_{\mathrm{a}}\left(\frac{1}{T_{\mathrm{refa}}}-\frac{1}{T}\right)\right)}_{\dot{D}_{\mathrm{a}}}$$

Numerical solution of the damage differential equation:

`*usermat`



$D_{\mathrm{ca}} = 0$ initialization

$\dot{D}_{\mathrm{ca}} = \dot{D}_{\mathrm{c}} + \dot{D}_{\mathrm{a}}$

num. integration

D_{ca}

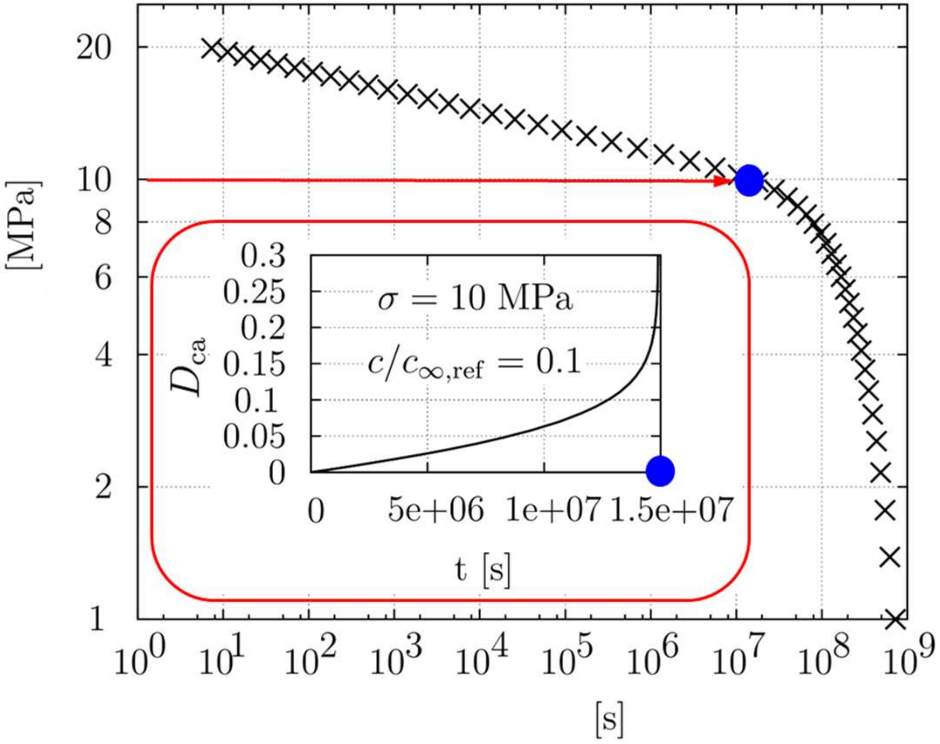
$D_{\mathrm{ca}} < 1$?

yes

no

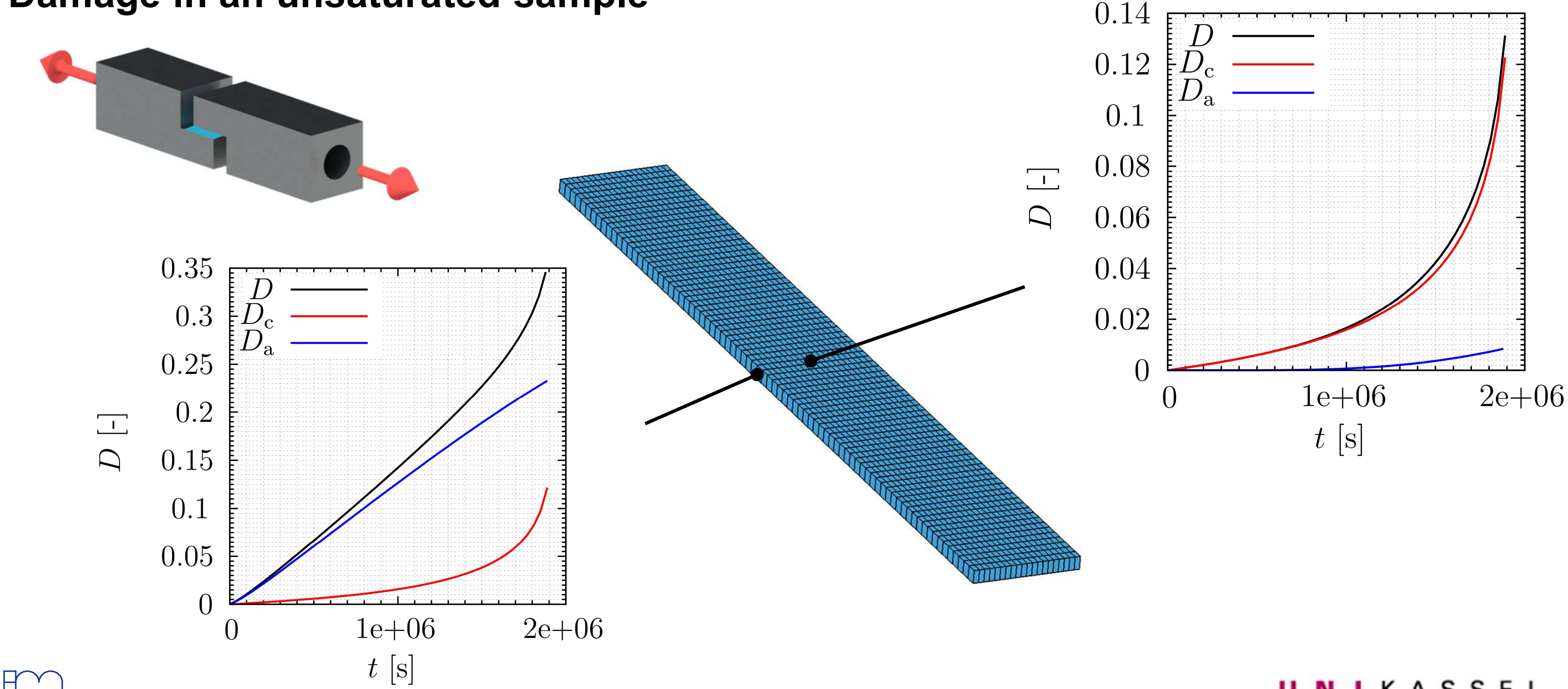
time of rupture ✕

or ● for $\sigma = 10$ MPa



Solution with LS-DYNA: Hygro-thermo-mechanical damage

Damage in an unsaturated sample



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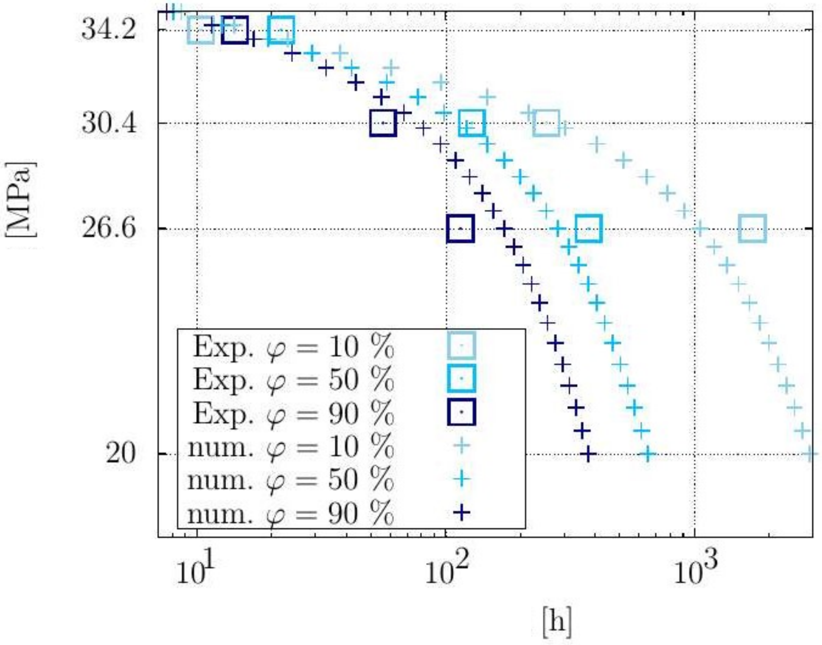
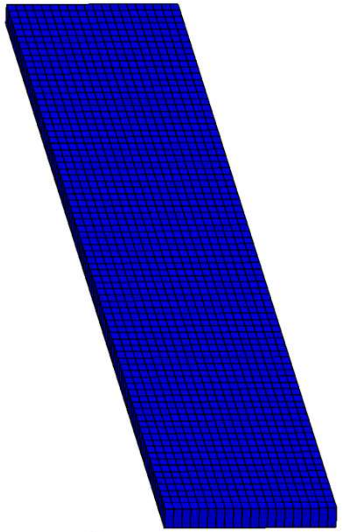
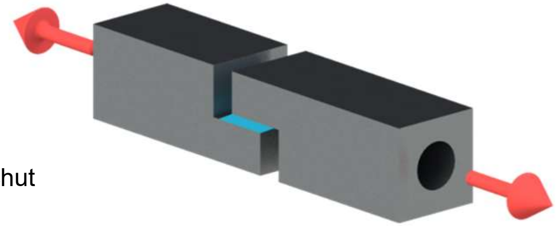
FE-Calculation and lifetime prediction under hygro-thermo-mechanical influences: Verification

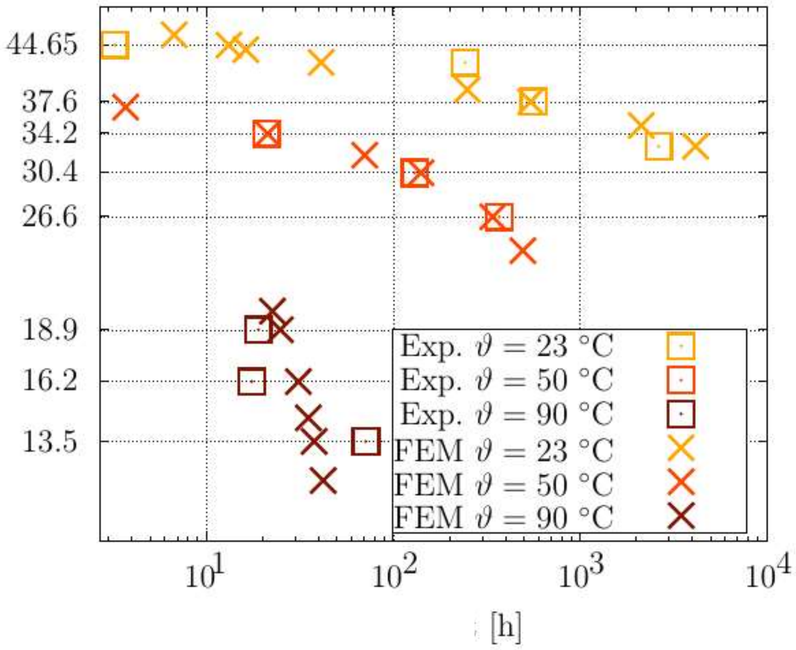
Tensile shear test under creep load at different temperatures and relative humidities

Comparison with experiment: good agreement









[1] Laboratorium für Werkstoff und Fügetechnik, Paderborn, Prof. Meschut

16. LS-DYNA Forum 2022

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Fabian Kötz, Anton Matzenmiller

Method Development: Characterization, Modeling and Simulation of Hygro-Thermo Effects in Thick Layer Adhesives

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