Modeling and Simulation of the long-term Behavior of Thermoplastics in LS-DYNA

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1 Abstract

Viscoelasticity respectively the time-dependent and the recovery behavior plays an essential role, especially for polymers. Nowadays, it is becoming increasingly important to be able to make service life predictions and forecasts regarding the long-term behavior of components using simulation models. In this context, constant or cyclic loads are usually the decisive mechanisms for deformation.
Moreover, the short-term behavior of plastics is also strongly characterized by viscoelastic phenomena. Even in the case of very short-time high loads on polymer components, the corresponding recovery behavior is of great importance and must be correctly represented in the simulation.
Material and simulation models must take this long-term but also the short-term behavior into account for a realistic prediction of the deformation behavior in order to be able to make corresponding estimates of the service life of components, which is often designed for years. For this purpose, this behavior must be characterized in the application-specific framework and considered accordingly in the modeling.
This article will present and compare some of the currently available material models that can account for the viscoelastic or time-dependent behavior of polymers, as well as the possibilities and effort required to obtain the material data needed for simulation.

2 Introduction

Numerical simulation for the virtual investigation of real problems has become established in the past and simulation is becoming more and more important in all industries. In the case of polymers, the viscoelastic behavior plays a particularly important role. Nowadays, it is becoming increasingly important to be able to make service life predictions and forecasts regarding the long-term behavior of components

Fig. 1: Simulation models for determining the long-term behavior for polymer components

using simulation models. Here, mostly constantly occurring or cyclic loads play a major role. For example, in tool making or in the microelectronics industry [1] or for facade fastening anchors, as shown in Fig. 1. This fastening system is used to fix facade panels to house walls. This results in a permanent load on these anchors. Here, the long-term behavior is of course of great interest, i.e. how this anchor will behave in a few years, so that it can be guaranteed that the facade panel will still be in place for instance in 20 years.
Moreover, the short-term behavior of polymers is also strongly influenced by viscoelastic phenomena, and i.e. the corresponding time-dependent recovery behavior is some times of great importance even for very short-term high loads and must be correctly reproduced in the simulation.
Material models have to take this behavior into account for realistic prediction. For this purpose, this behavior must be characterized in the application-specific framework and also considered in the modeling. Subsequently, material models are considered that can account for the viscoelastic behavior

or the time-dependent behavior of polymers and their respective limits are estimated. In addition, it is also important to determine the material data for modeling with as little effort as possible and to have a methodology for modeling the material behavior.
Mechanical stress on a thermoplastic cause both reversible and irreversible deformations. In most cases, the individual areas are described in the literature on the basis of stress-strain curves, as shown in Fig. 2a [2]. Here, it is assumed that at small strains the entire deformation behavior is time-dependent,

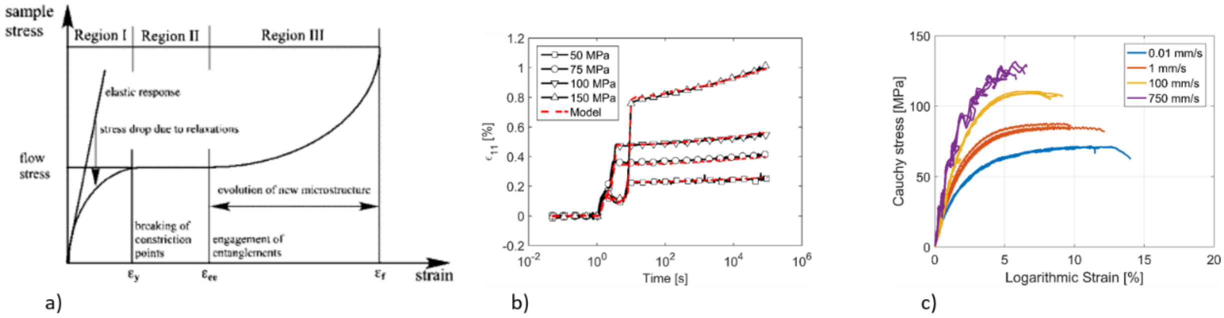


Fig. 2: Mechanical response of thermoplastics; a) Schematic overview with regard to the stress-strain behavior [2]; b) Creep behavior at different load levels [3, 4]; c) Strain rate dependency [5]

but completely reversible divided into linear, i.e. independent of the stress level, and non-linear, meaning that in addition to the time-dependent recovery behavior, the corresponding stress level also plays a role. At higher stress levels, plastic and thus irreversible deformations then occur. Viscoelasticity now describes both elastic and viscous behavior, with the usual suspects here being creep behavior, relaxation and strain rate dependence, which is also mainly caused by viscoelastic and not viscoplastic effects, Fig. 2b, c [3–5]. Therefore, this article provides an overview and also a comparison of material models available in LS-Dyna to describe the short-term but also long-term effects and concludes with an outlook on a model that follows a multiple natural configuration approach.

3 Characterization

What was observed in experiments all over the years is, that even with near-failure loading or a high degree of fiber orientation the mechanical behavior is predominantly viscoelastic not depending on the strain rate. Usually it is assumed that the behavior at small strains or deformations is reversible, i.e. linear or non-linear viscoelastic.

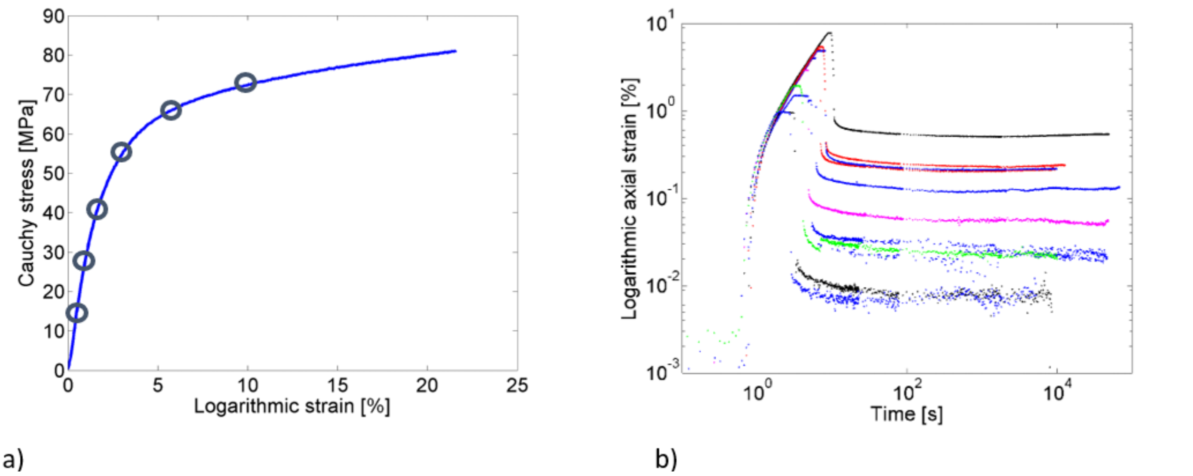
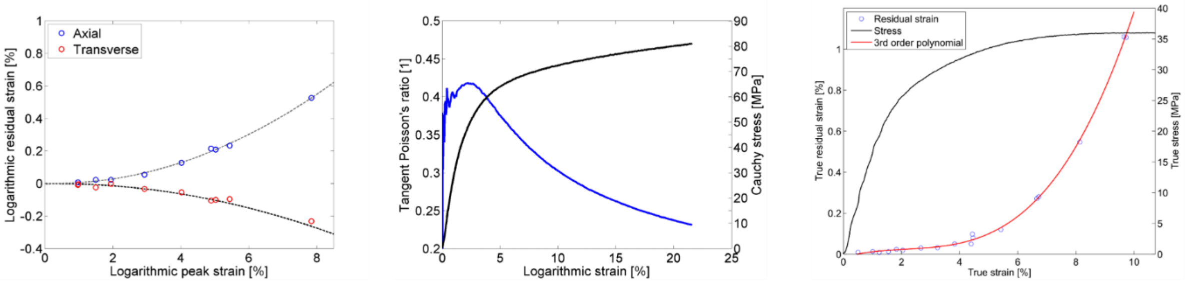


Fig. 3: Strain-Recovery Method; a) Schematic creep loads for strain-recovery measurements; b) Creep-recovery behavior

One possibility to make more precise statements here is the so-called strain recovery method [6]. This method starts with a mechanical test with DIC for strain recovery, e.g. monotonic tests (tensile, compression or bending tests or similar, creep, relaxation, cyclic tests, etc.). After that, the stressed specimen is unloaded by releasing the clamping dies or by machine-controlled unloading and the

recovery strain is measured directly on the respective test rig during the first minutes. In the third step, the specimens are moved to a recovery test rig and are continued to be measured optically.
Fig. 3 shows for example creep tests carried out at different stress levels according to the stress-strain curve Fig. 3a), there are different time-dependent deformations and correspondingly serious differences in the residual strains Fig. 3b). And it is obvious that even with quite small loads and correspondingly low strains, an irreversible deformation component already remains. Regarding the time component it can be said that there is no general statement regarding how long a material will recover, since this depends strongly on the respective material. While POM, for example, almost reaches a steady state after ~20 minutes, this is only the case with PP after ~24 hours.



a) b) c)

Fig. 4: Determination of irreversible strain; a) Evolution of residual strain with time; b) Tangent Poisson's ratio describing the total strain behavior; c) Residual strains after recovery

It is therefore difficult to separate reversible and irreversible deformation in thermoplastics. In Fig. 4a one can see that even at quite low strain levels there is a proportion of residual strain, which increases nonlinearly with an increase in the total strain. Comparing the plastic behaviour, Fig. 4a, with the total strain behavior, Fig. 4b, represented by the tangent Poisson's ratio, it is obvious that the plastic strain exhibits a fairly constant transverse contraction behavior due to deviatoric plastic deformations, whereas this effect does not apply to the total strain due to the volumetric components.
Nevertheless, it can be concluded from Fig. 4c that a large portion of the strains that occur are reversible, since the plastic strain accounts for only about 10% of the total strain, even near the failure strain. Thus, it can be seen that the time-dependent recovery behavior of thermoplastics in simulation are essential to describe them. This can be achieved by performing creep tests.

a) b)

Fig. 5: Devices for creep testing; a) Self constructed 5-fold creep test rig; b) Anton Paar DMA MCR 702e MultiDrive

One possibility for the realization of creep tests are classical short-time creep tests or alternatively the so-called Stepped Isothermal Method as an accelerated method. To carry out the classical variant, a self-constructed creep test rig can be used at PCCL, Fig. 5a, whereby the load application can be carried out separately for each specimen via levers and dead weights. With the aid of a temperature chamber and an air conditioning unit, isothermal tests can be carried out in a temperature range from -5°C to 250°C, with strain measurement in the longitudinal and transverse directions being performed optically via digital image correlation. The specimens are heated to the respective temperature in advance. This allows a very uncomplicated determination of the creep behavior, since no thermal effects have to be taken into account during the actual creep tests. As an alternative to the classical short-time creep tests, which can be very time-consuming depending on the desired temperature range, accelerated measurement methods based on the Boltzmann superposition principle have emerged in the past. One of these accelerated methods is the so-called Stepped Isothermal Method, or SIM for short, which can be conducted using a DMA, see Fig. 5b, for example. Here, the time-dependent strain behavior at different temperature levels is measured continuously on one and the same test specimen in one and the same test. The great advantage is that only one test specimen is required for all temperature levels. However, this method has the major disadvantage that the thermal strains must be extracted from the

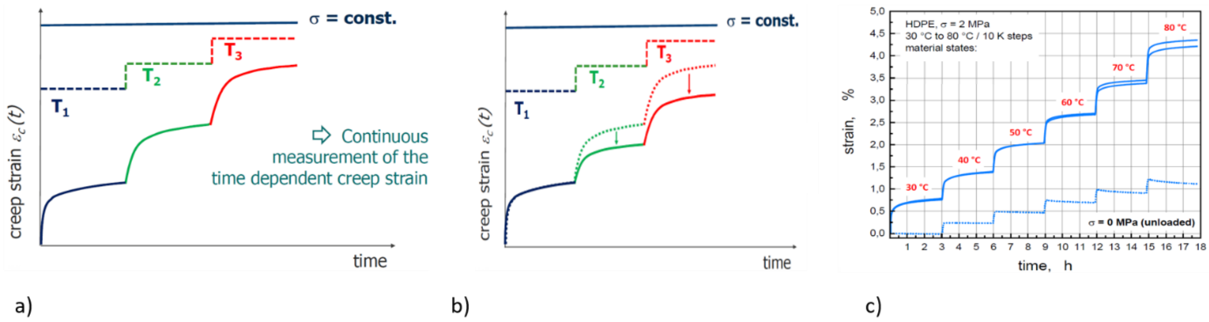


Fig. 6: Illustration of the Stepped Isothermal Method; a) Measurement of the creep strain; b) Subtracting thermal strains; c) Example of resulting creep curves [7]

creep strains, since these do not originate from a mechanical background. Therefore, one has to perform a 0-load test with exactly the same temperature profile as for the other measurements in order to subtract these thermally induced strains from the total strain to obtain a purely mechanical behaviour, Fig. 6. A more detailed discussion on this topic can be found in [7].
As part of the research work, various thermoplastic materials were characterized and the corresponding creep behavior determined. The results for a PE loaded at 5 MPa are shown in Fig. 7.

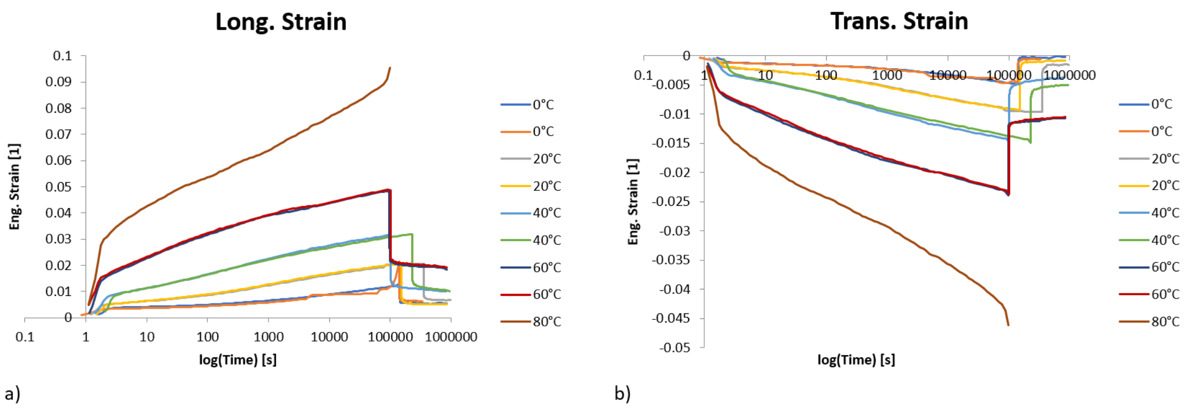


Fig. 7: a) Creep behavior at 5 MPa load of PE in longitudinal direction; b) Creep behavior at 5 MPa load of PE in transverse direction.

4 Modeling

In the linear deformation domain, one can refer to the Boltzmann superposition principle, which states that there is no coupling or interaction between the loads.

$$\sigma(t) = \int_{0^-}^{t} E(t-\tau)\frac{\partial \varepsilon_x(\tau)}{\partial \tau}\,d\tau \qquad (1)$$

Please note that this is only true in the linear domain. That is, the reaction caused by multiple loads can be equated to the sum of the reactions that each individual load level would attempt. Thus, if a linear material is loaded at 1 MPa and after a certain time a weight is added and the material is suddenly loaded at 2 MPa, the resulting strain will be equal to the sum of the strains if the two loading levels had been tested separately. The viscoelastic response is thus theoretically built up via the response to a step load. If one considers the limiting case of an infinite number of such infinitesimal steps, one obtains

a general representation of the time-dependent behavior, represented in the integral equation of Equ.1, which says nothing other than that the stress at time t arises from the strain evolution up to this time. And in order to be able to capture this numerically, one needs a mathematical expression for the time-dependent modulus, which is usually achieved by means of mechanical substitute models, i.e. spring-damper models.
These spring-damper models can represent different time-dependent phenomena according to their definition. With the help of the Kelvin-Voigt model, for example, the creep behavior can be represented and with the help of the Maxwell model the relaxation behavior. What both models cannot do, however, is to represent the recovery behavior as well, due to their damper components. Additional models must be defined which also consider possible recovery behavior. For this purpose, the standard linear solid model (SLS model for short) is used to arrive at the generalized representation from spring-damper models, which describe the compliance behavior in the discrete using a sum representation, see Equ.2.

$$J(t) = \frac{\sigma(t)}{\varepsilon_0} = J_\infty - \sum_{i=1}^{N} J_i e^{-t/\tau_i} \tag{2}$$

This representation also corresponds to the solution of the differential equation. This is because in the time domain, the solution of the differential equation is a sum of exponentially decaying relaxation terms. For this generalized model, N non-linear and N+1 linear parameters have to be determined and in practice they are optimized, for example, using least squares optimization, or using iterative algorithms such as Gauß-Newton-method, or stochastic algorithms such as Simulated Annealing.
In most FE solvers, also in LS-Dyna, the viscoelastic behavior is usually incorporated via relaxation models. Here, the viscoelastic behavior is additively separated into a linear elastic part described by the inverse stiffness matrix and a corresponding time-dependent part defined by a Prony series expansion, see Equ. 3.

$$\boldsymbol{\varepsilon} = \boldsymbol{D}^{\mathbf{0}}\boldsymbol{\sigma} + \int_{0^-}^{t} \Delta\boldsymbol{S}(t-\tau)\frac{\partial\boldsymbol{\sigma}(\tau)}{\partial\tau}d\tau \tag{3}$$

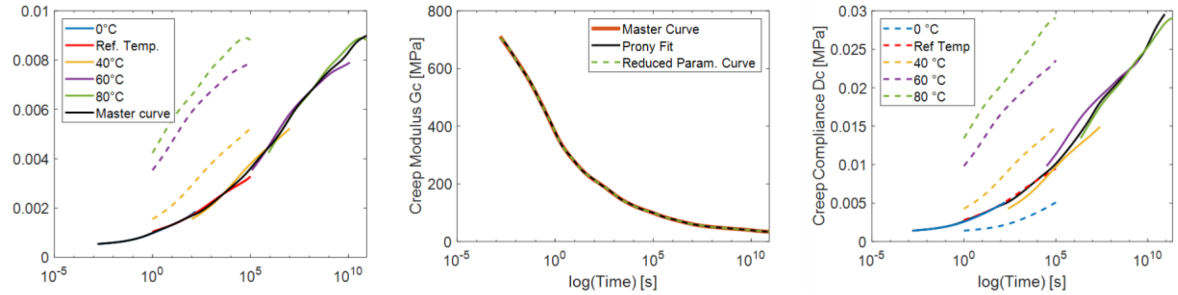
As mentioned at the beginning, both the volumetric and the deviatoric part play an important role for the description of the long-term behavior. Therefore, also the most common solvers offer the possibility to define both the compression behavior - to describe the volumetric behavior, and the shear or tensile behavior to describe the deviatoric behavior. However, as already described here, it must be taken into account whether the short-time modulus or the long-time modulus is used to describe the elastic behavior, because the definition of the time-dependent moduli then differs fundamentally from one another.

In LS-Dyna there are several possibilities to consider viscoelasticity in the simulation. Two of them will be discussed and compared in this paper. On the one hand the model ***MAT_076** and on the other hand the new add on model ***MAT_ADD_INELASTICITY** (short **MAI**) was examined. The viscoelasticity is realized in both models via a Prony series expansion, see Equ. 4. Elastic parameters must be defined to describe the instantaneous modulus, although these play a minor role in ***MAT_076** and have almost no effect on the simulated behavior. The situation is different when the model **MAI** is coupled with the model ***MAT_002**. Here, the level of the strains, as well as the transverse contraction behavior can be significantly influenced via the elastic parameters.

$$g(t) = \sum_{m=1}^{N} G_m e^{-\beta_m t} \tag{4}$$

In general, the effort for model calibration is similar for both models, since besides the number of Prony terms N, one only has to adjust the corresponding parameters G_m and β_m, see Equ. 4.
For the inclusion of the temperature dependence LS-Dyna offers two possibilities with an Arrhenius and a WLF formulation (Arrhenius 1-parameter model and WLF a 2-parameter model), with the WLF formulation being more appropriate for describing the temperature behaviour.
At the end of the day, however, comparable results are obtained with both models, as shown in Fig. 11.

Next, a possible strategy for deriving the model parameters from test data is described. If the long-term behavior is relevant and one has test data at different temperatures, one can generate a master curve with respect to the creep compliance via the time-temperature shift principle, see Fig. 8a. Thus, one has defined a description of the long-term behavior of the material over several decades based on a few short-term tests. This master curve then serves as a basis for optimizing the parameters of the Prony series expansion shown in the previous slide, see Fig. 8b. Thus, one has incorporated the entire material behavior over the time span defined in the master curve into the material model. If required, a temperature dependence remains to be included, and this is also done by optimizing the corresponding parameters of the Arrhenius or WLF formulations, see Fig. 8c. So, the entire material model for the viscoelastic behavior has been defined. What is still missing are the elastic characteristic values, which can either be determined directly from the creep data, or quasi-static tensile tests are additionally carried out to determine these, which in principle leads to the better results, because when using the creep data to determine the elastic behavior, optimization of these parameters is usually necessary.



a) b) c)

Fig. 8: Determination of model parameters; a) Generation of a master curve; b) Prony-parameter optimization using e.g. nonlinear least squares method; c) WLF-parameter optimization using e.g. nonlinear least squares method

5 Validation and Application

For verification of the defined model validation simulations were performed on specimen level. A model of the free-moving part of the specimen was created and meshed with fully integrated Solid-Hex elements, see Fig. 9. As boundary conditions, homogeneous Dirichlet boundary conditions simulating the pinching behavior were applied to the upper side of the specimen and the corresponding temporal load curve from the test - which, with the exception of the load range, is virtually constant over the entire course of the test - was applied to the lower side of the specimen. Of course, an implicit time integration was chosen due to the long simulation times. The strain evaluation of the simulations was performed in the parallel area of the specimen according to the DIC evaluation of the tests. To apply the temperature in combination with a time-temperature shift (e.g. WLF), a system reference temperature must be defined. The use of ***LOAD_THERMAL_CONSTANT** is therefore not recommended, since no system reference temperature can be defined there. Instead, the temperature load should be included with the keyword ***LOAD_THERMAL_VARIABLE**, because a reference temperature can be specified there, which is essential for the definition of the elastic parameters at the specific reference temperature.

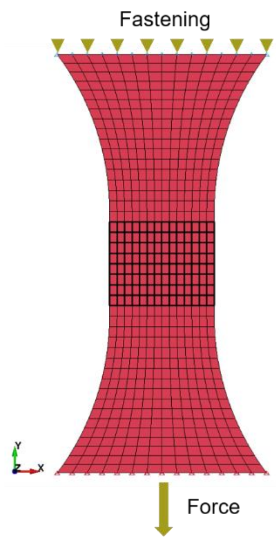


Fig. 9: Simulation model

As one can see in Fig. 11, both models reproduce the material behavior quite well. The simulation times of the two models are also almost identical. The measurable difference is only influenced by the number of background processes. Parallelization works very well with both models and leads to a reduction of the computing times almost by a factor similar to the processors used. What was noticed with both models, however, is that the time-temperature shift is very cost-intensive and increases the further one moves away from the reference temperature. Here, it can already lead to significantly longer computing times. With the validated models, a component simulation was subsequently carried out on the basis of such an insulation board anchor, see Fig. 11a. The top of the anchor was fixed according to the real load case and the corresponding force was applied to the nail. The resulting strain was measured in a rather simplified way via the deformation movement between two points.

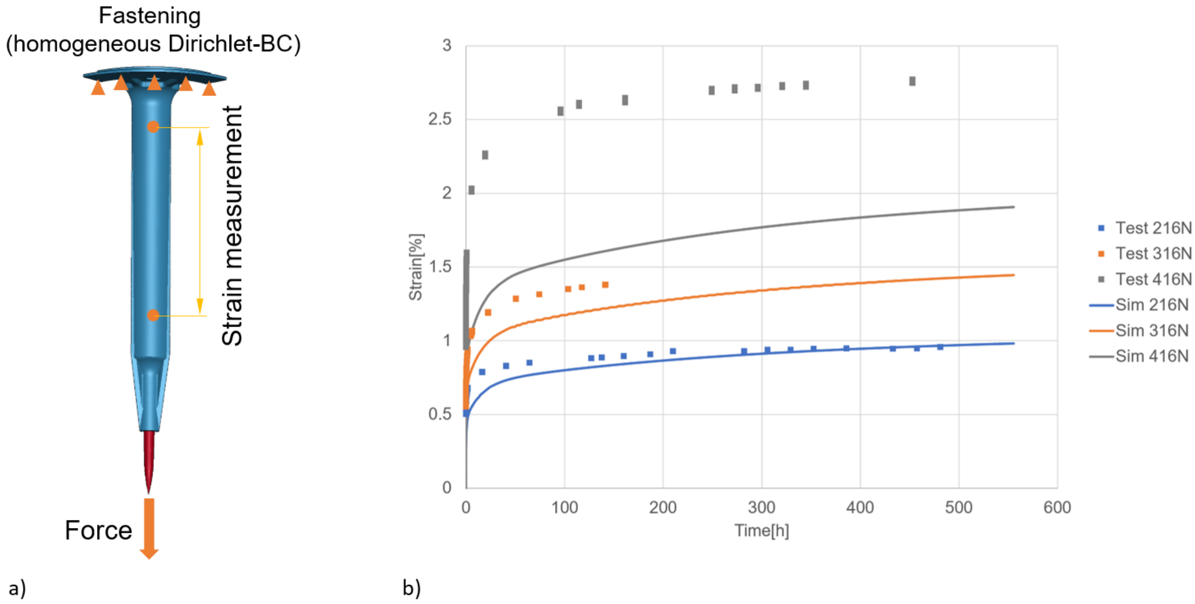


Fig. 10: Validation model and results on component level; a) Simulation model of an insulation board anchor; b) Simulation results using a linear viscoelastic model corresponding to 216N loading

Three different load levels were measured, with the lowest load level corresponding approximately to that from the tests. As can be seen in Fig. 11b, the lowest load level is still represented quite well, but with increasing static load and the onset of nonlinearity, the behavior can no longer be reproduced with the models used, i.e. one must either use nonlinear models or linear models at the corresponding load levels. Linear models are usually sufficient for known and constant loads and can be characterized and

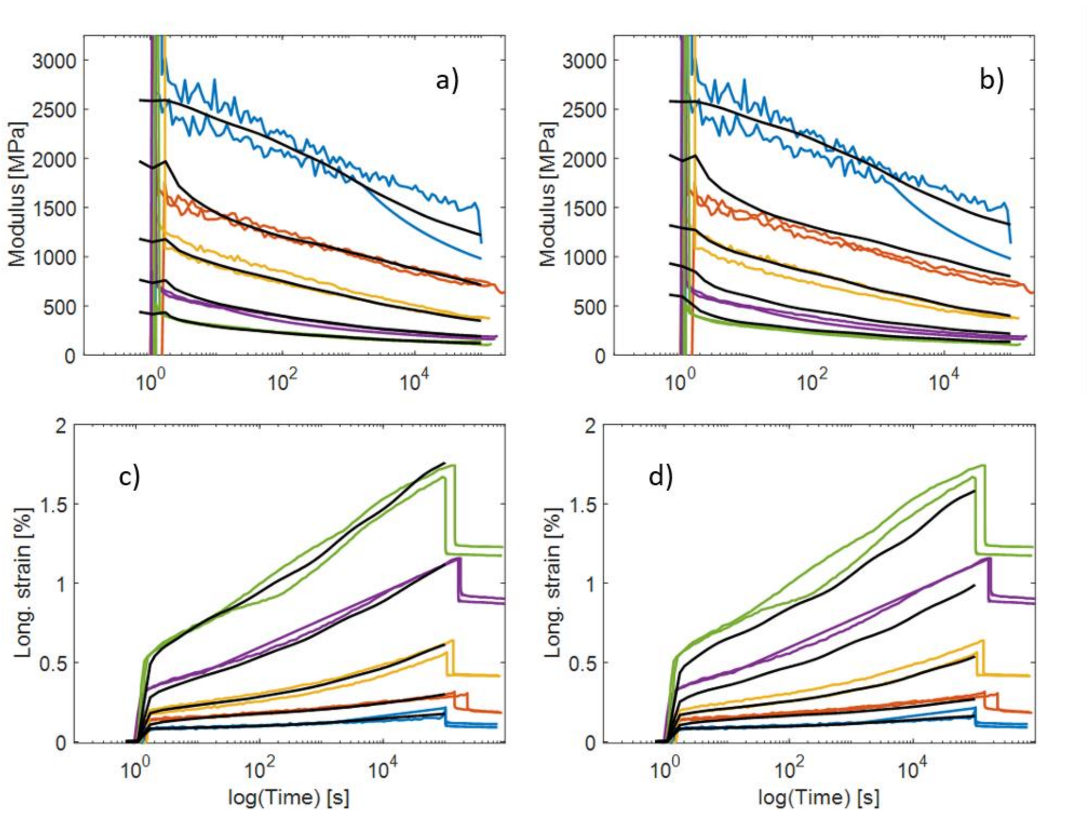


Fig. 11: Verification results on specimen level; a) ****MAT_076*** *prediction of the creep modulus; b)* ****MAT_002+MAI*** *prediction of the creep modulus; c)* ****MAT_076*** *prediction of the strain behavior ; d)* ****MAT_002+MAI*** *prediction of the strain behavior*

adapted with relatively little effort. However, if load fluctuations occur or different constant loads occur, one must switch to nonlinear models.

6 Summary and Outlook

Methods for characterizing long-term behavior using classical creep tests and the Stepped-Isothermal Method were presented. Furthermore, an insight into linear viscoelastic modeling as performed in LS-Dyna was given and a possible approach to calculate the model parameters was shown. The calibrated models were validated and compared with each other in terms of prediction quality and computation time. Finally, the respective limitations of the models were presented by means of a validation example. Finally, a short outlook on the nonlinear modeling of viscoelastic effects using a multiple natural configuration approach is sketched here.

Starting point for this approach is that the macroscopic response of materials to mechanical stresses, which are often described in terms of constitutive relationships, reflects the changes that take place in the microstructural morphology of the material. The macromolecular structures of polymers affect their mechanical and physical properties, and thus their overall performance, when exposed to external stimuli. For example, polymers can undergo various microstructural changes, e.g., scission, crazing, entanglement, fragmentation, etc., when it is subjected to a mechanical load. And this results in a nonlinear and inelastic behavior. The viscoelastic behavior here is attributed to the motion of long chains (macromolecules), which is strongly influenced by the loading history. For example, the long chains may rearrange, reorient, break (scission), slip, or something like that, when the polymer is subjected to a sufficiently long mechanical load, and after the mechanical load is removed and even with sufficient recovery time, the polymer may not regain its original macromolecular structure, resulting in permanent deformation on the macroscopic scale, see Fig. 12, [8, 9], which was already shown in the strain recovery approach.

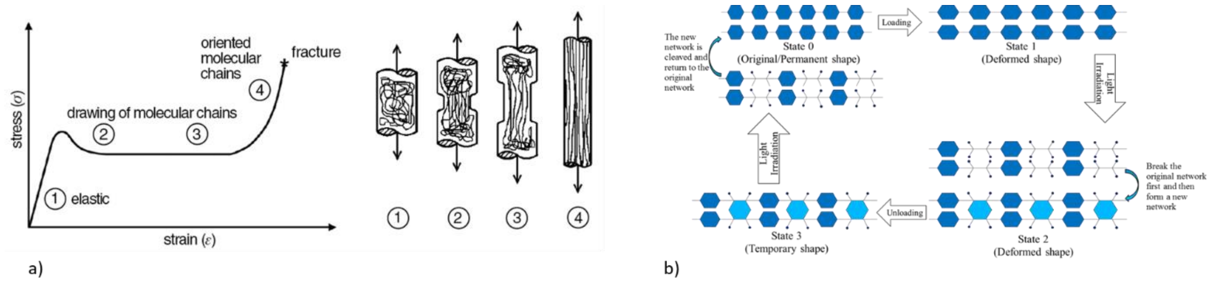


Fig. 12: Stress-strain behavior of thermoplastic polymers during tensile testing

The considered model allows the description of the mechanical response of viscoelastic polymers undergoing microstructural changes considering several natural configurations, see Fig. 13. In order to consider the effect of microstructural changes on the macroscopic response of polymers, it is assumed that the considered polymer consists of two networks.

$$\boldsymbol{\sigma} = \boldsymbol{C}_0 \boldsymbol{\varepsilon} \quad (5)$$

In its initial configuration, the polymer is composed of an original microstructure (initial network, Equ. 5) and when the polymer is deformed, a new network is formed.

$$\boldsymbol{\sigma} = \boldsymbol{C}_f \boldsymbol{\varepsilon} \quad (6)$$

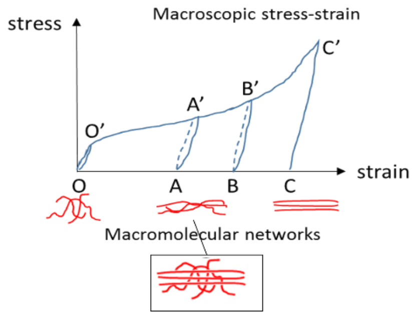


Fig. 13: Multiple Natural Configuration Approach

The newly formed network has a new reference configuration, see Equ. 6. When subjected to mechanical stress, the natural configuration of the polymer evolves between these initial and final configurations, see Equ. 7.

$$\boldsymbol{\sigma} = \boldsymbol{C}\left(\boldsymbol{C}_0, \boldsymbol{C}_f, \alpha\right)\boldsymbol{\varepsilon} \quad (7)$$

For a more detailed description of this model it is referred to [9, 10] .
Currently, the model is implemented only with an analytical solver in MatLab, but initial simulation results showed very good agreement of the simulated data with the experimental one over a wide range of loads, as shown in Fig. 14 and Fig. 15. In a next step, this model will be implemented in a commercial FE software on the part of the partner Texas A&M.

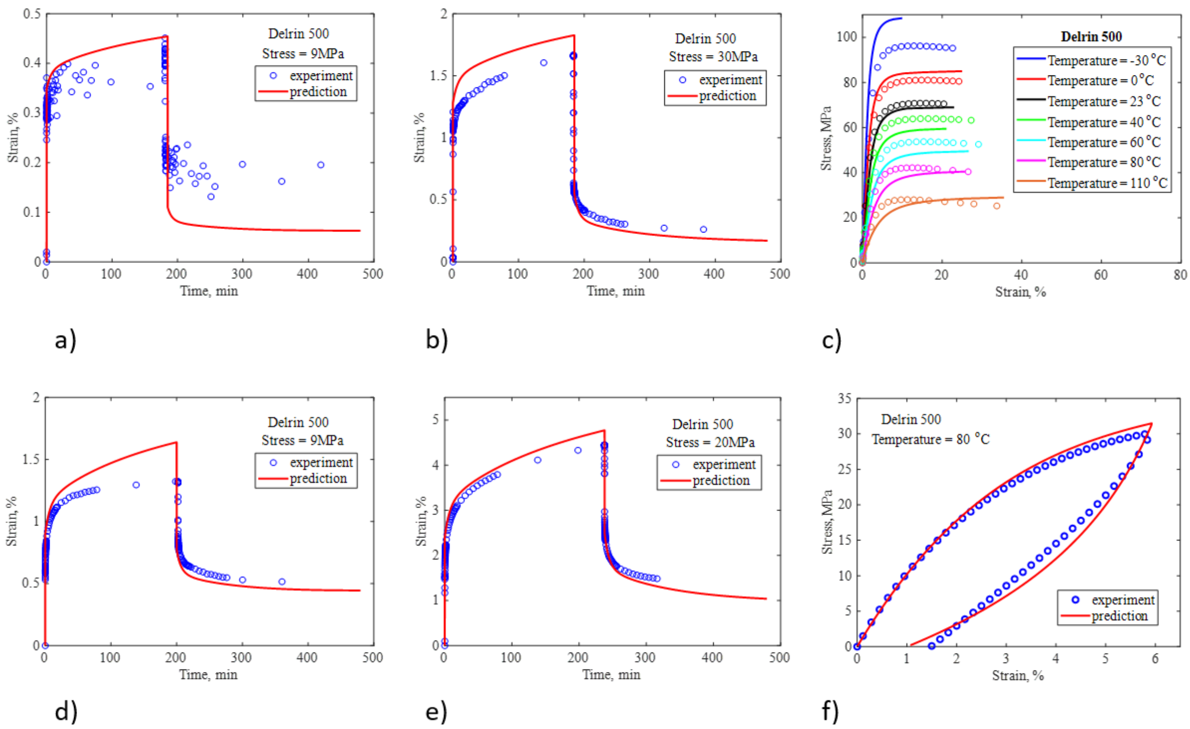


Fig. 14: Validation simulation nonlinear model; a) Creep-recovery at 23°C and 9MPa; b) Creep-recovery at 23°C and 30MPa; c) Creep-recovery at 80°C and 9MPa; Creep-recovery at 80°C and 20MPa; e) Tension; f) Loading-Unloading [10]

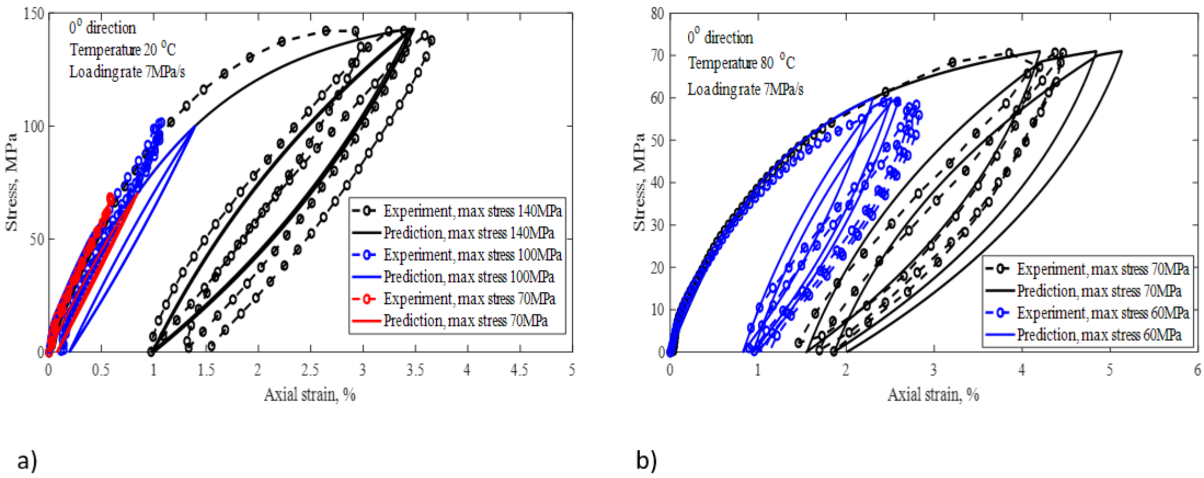


Fig. 15: Loading-Unloading behavior at a) room temperature and b) 80°C using the nonlinear model approach

7 Literature

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