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Computational analysis of PTFE shaft seals

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Abstract

An endochronic viscoplastic approach, derived from the theory of finite viscoplasticity based on material isomorphisms, is presented, in order to describe the nonlinear material behaviour of filled polytetrafluoroethylene (PTFE) in a computational analysis of PTFE shaft seals. The model allows to characterize viscoplastic material behaviour with an equilibrium hysteresis using a rate-independent elastoplastic model (with an endochronic flow rule and a logarithmic elastic law) in parallel connection with a nonlinear Maxwell model. Due to the endochronic flow rule, an elastic range limited by a yield stress is not needed in the present approach. The volumetric stress contribution is assumed to be purely elastic. The proposed model is applied to simulate the mounting process of PTFE shaft seals in an axially symmetric finite element analysis. The numerical results (radial force, pressure in the contact zone) are in fair agreement with the experimental data.

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1. Introduction

Due to their tribological characteristics, chemical inertness and temperature stability, PTFE compounds are increasingly used in engineering, especially for rotary shaft seals. However the engineer has to take into account the viscoplastic mate-

rial behaviour of PTFE which is radically different from that of elastomeric materials used in classical rotary shaft seals.

In order to prepare a numerical simulation of the sealing system, uniaxial experiments have been carried out to study the mechanical behaviour of a typical PTFE compound that consists of 90% PTFE and fillers (5% short cylindrical glass fibres and 5% MoS₂). These fillers are used to improve the performing properties of PTFE. Glass fibres reduce the wear of the seal. MoS₂ decreases the friction between the seal and the shaft in the contact zone.

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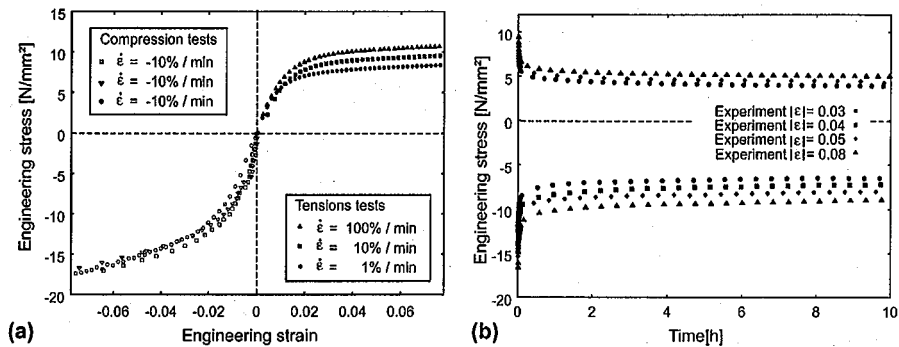


Fig. 1. Experimental data of uniaxial tests in tension and compression. (a) Strain-rate-dependence and SDE, (b) stress relaxation in tension and compression.

The material behaviour of this special compound has been intensively studied in uniaxial tests (tension tests at different strain rates, stress relaxation and retardation), see [14,11,9]. Experimental data of these investigations are shown in Fig. 1. Due to these observations a successful constitutive approach to this class of materials must be able to predict the following effects:

- strain-rate-dependence during loading;
- stress relaxation at constant strain;
- strain recovery in the unloaded state;
- plastic deformation;
- asymmetric material behaviour in tension and compression (SDE—strength differential effect).

In the past, engineers used different constitutive laws for numerical simulations of different processes. The mounting of the seal on the shaft (short time process) was usually calculated using an elastoplastic, [15,14], or a viscoplastic approach with a strain rate dependent yield stress [14]. Viscoelastic approaches were applied to analyze the stress relaxation (long time process) in a mounted seal.

An additive decomposition of the total stress into a rate-independent equilibrium stress and a rate-dependent overstress can be found in the calculations of Wüstenhagen [17] and Lin [13]. The linear viscoelastic approach of Wüstenhagen [17] is limited to very small strains. The more sophisticated theory of finite linear viscoelasticity, used by Lin [13], allows to regard physical and geometrical nonlinearities at different constant temperatures

during the computation, but the rate-independent plastic deformation (that can be clearly observed during the tests) and the SDE remain unconsidered by the use of these purely viscoelastic approaches.

In order to simulate PTFE shaft seals successfully in a unified approach without neglecting important inelastic effects that are clearly detected in the experiments and without jumping from one constitutive law to an other, this paper presents the application of the endochronic viscoplastic material model (proposed by Kletschkowski et al. [9]) to the computational analysis of PTFE shaft seals. The endochronic theory of plasticity was developed by Valanis [16] and is discussed in detail in Haupt [7,8] and Krawietz [12].

2. Finite viscoplasticity based on material isomorphisms

The investigated PTFE compound is a typical example of semi-crystalline polymers. The mechanical strength of these materials is based on the strong cohesion of the molecules inside the crystallites. Semi-crystalline solids derive their flexibility from the mobility of the molecules outside of the crystallites (inside the amorphous phase). The preponderant part of the reversible deformations is based on the processes of sliding molecules inside the amorphous ranges. The evolution of irreversible plastic strains is associated with the stretching of the crystallites.

In order to describe this deformation behaviour a phenomenological model has been proposed by Kletschkowski et al. [9]. This approach is capable to characterize the viscoplastic properties of semi-crystalline PTFE compounds using a nonlinear rate-independent endochronic elastoplastic model in parallel connection with a nonlinear Maxwell model. The deformation of the amorphous ranges is characterized by the Maxwell model. The endochronic model has been introduced in order to describe the plastic deformation of crystallites. Hence this kind of macroscopic modelling is basically inspired by the physical causes of the phenomena to be described below.

Nevertheless, in contrast to micro-mechanical models based on polymer physics [1,2,5] the presented approach is established on the macro-level. Still, it is possible to emphasize some advantages of our approach when taking the special characteristics of the investigated material into account.

Material models for rubber-like solids (e.g. [1,13]) are not capable of describing the viscoplastic behaviour of semi-crystalline solids. This is caused by the asymmetric stress–strain-characteristic, generated by these approaches, in order to model the nearly incompressible material behaviour of rubber elastic solids. In contrast to this, in simple tension and under simple compression the stress–strain behaviour of pure PTFE is nearly identical, as mentioned in [14].

The stress–strain-asymmetry of glass fibre filled PTFE is caused by the introduction of the filler particles. Hence, in order to describe the behaviour of the PTFE-matrix, the starting point should be a material model that generates a symmetric stress–strain-behaviour in tension and under compression in the absence of filler particles.

The approach suggested by Arruda and Boyce [2] has been successfully applied to the elastic-viscoplastic deformation behaviour of glassy amorphous polymers. Hence, the prediction of the stress drop after reaching the region of the fully developed viscoplastic flow, as well as the strain-hardening behaviour of glassy polymers at finite strains, is excellent. But, the application of this approach to semi-crystalline PTFE-materials would result in an underestimation of the reversible parts of the deformation. Furthermore, a stress

drop (after reaching the flow region) has not been observed in the experiments as illustrated by Fig. 1.

The model presented by Drozdov and Christiansen [5] is a successful application of a micro-mechanical approach to the elastoplastic material behaviour of semi-crystalline isotactic polypropylene. Unfortunately, the strain-rate-dependence of these class of materials has not been included in this concept up until now. Furthermore, in order to be in consistency with the second law of thermodynamics, two plastic strains have been introduced. The second plastic strain develops only during unloading. Therefore, active loading and unloading has to be distinguished in the approach presented by Drozdov and Christiansen [5].

The concept suggested in the present paper describes the equilibrium hysteresis of semi-crystalline materials using only one plastic variable. Furthermore, we do not need to distinguish between active loading and unloading in the presented unified approach.

The theoretical background of the endochronic viscoplastic material model for filled PTFE, proposed by Kletschkowski et al. [9], is given by a modification of Bertram's approach to finite plasticity based on material isomorphisms, see [3,4]. First the fundamental ideas of this concept will be summarized.

The approach starts with the definition of the independent and the dependent variables of a deformation process. If \mathbf{F} is the deformation gradient and \mathbf{T} the Cauchy stress tensor, then $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ defines the right Cauchy–Green tensor and $\mathbf{S} = \mathbf{F}^{-1} \mathbf{T} \mathbf{F}^{-T}$ the material stress tensor. \mathbf{S} is work-conjugated to \mathbf{C}

$$\text{tr}(\mathbf{T}\mathbf{L}) = \frac{1}{2} \text{tr}(\mathbf{S}\dot{\mathbf{C}}) \quad \text{with}$$

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1} \quad (\text{spatial velocity gradient}). \quad (1)$$

An elastic range $\{E_p, h_p\}$ is defined as a path-connected subset E_p of the configuration space, which forms a differentiable manifold with a boundary [3]. h_p is the elastic law in the elastic range E_p . This approach to finite plasticity is completed by the assumptions that

- the material is within an elastic range at any time;
- the elastic range is only changed during an inelastic deformation process;
- the elastic laws of all elastic ranges of the material are isomorphic.

The change of the initial elastic range $\{E_0, h_0\}$ to the actual elastic range $\{E_p, h_p\}$ is described by an elastic isomorphism \mathbf{P} as

$$h_p(\mathbf{C}) = \mathbf{P}h_0(\mathbf{P}^T\mathbf{C}\mathbf{P})\mathbf{P}^T. \quad (2)$$

\mathbf{P} is called plastic transformation. Its properties are discussed in detail in [3]. For the evolution of \mathbf{P} , rate equations are proposed in the context of finite plasticity.

The endochronic viscoplastic material model for filled PTFE, proposed by Kletschkowski et al. [9], is based on Bertram's approach to finite plasticity. The following assumptions are needed additionally for the present approach:

- the material has isomorphic elastic ranges;
- the evolution of an inelastic transformation \mathbf{P} is determined by associated flow rules using a J_2 -theory of inelastic flow.

The constitutive model, used for the computational analysis of PTFE shaft seals, is summarized in Table 1. Its main features are the multiplicative decomposition of the right Cauchy–Green tensor \mathbf{C} into an isochoric and volumetric part (Eq. (3)) and the additive decomposition of the material stress tensor \mathbf{S} into a purely elastic stress, due to changes in the volume, a deviatoric equilibrium stress and a deviatoric overstress (Eq. (4)).

The volumetric stress is given by a nonlinear elastic law (Eq. (7)). An elastic model of the Neo–Hooke type (Eq. (8)) is applied to describe the overstress. The logarithmic elastic law of the endochronic model is given by Eqs. (9) and (10). K , G_{ov} , G_{∞} and B are the elastic constants of the model.

For the evolution of the viscous transformation \mathbf{P}_V a highly nonlinear flow rule of the Garofalo-type, see Garofalo [6], is applied (Eq. (11)). η , κ and σ_0 are constant model parameters. The evolution of the plastic transformation \mathbf{P}_P is determined

by a rate-independent endochronic flow rule (Eq. (13)), suggested by Krawietz [12]. Y is a constant stress type model parameter.

In order to consider the SDE, the internal variable D is introduced. Its evolution is determined by two saturation type evolution equations with respect to the permanent (Eq. (18)) and the non-permanent (Eq. (19)) characteristics of the stress–strain-asymmetry. K_i ($i = 1, \dots, 4$), D_p^{\max} and D_n^{\max} are constant model parameters. The details of this endochronic approach for materials with different behaviour in tension and compression will be published in Kletschkowski et al. [10].

The presented approach to finite viscoplasticity (Table 1) is suitable to describe finite inelastic deformations of isotropic materials without any constitutive decomposition of the independent variable \mathbf{C} into elastic and inelastic parts. Due to the Lagrangian approach, all time derivatives are material time derivatives. Hence all evolution equations and the elastic laws are objective. In general the inelastic transformations \mathbf{P}_P and \mathbf{P}_V are non-symmetric tensors. Therefore the inelastic spin is included into the concept. The Cauchy stress at any time can be easily calculated by a push forward operation $\mathbf{T} = \mathbf{F}\mathbf{S}\mathbf{F}^T$. The approach is valid for thermoplastic materials. In the present work the material parameters (Table 2) have been adjusted for the 10% compound by an indirect identification procedure using a uniaxial tension test at a strain rate of $\dot{\varepsilon} = 10\%/min$ and the succeeding stress relaxation at $\varepsilon = 8\%$ (ε denotes the engineering strain) and a uniaxial compression test at a strain rate of $\dot{\varepsilon} = -10\%/min$ and the succeeding stress relaxation at $\varepsilon = -8\%$. Details of this identification procedure can be found in Kletschkowski et al. [9,10].

3. Numerical investigations on PTFE shaft seals

In order to perform numerical simulations of PTFE shaft seals the presented model has been implemented into the USERMAT subroutine of the FE-Program ANSYS 6.1.

Axially symmetric solid elements (SOLID182) have been used to create the mesh of the seal. The shaft has been modeled by bar elements

Table 1

Constitutive equations at finite strains

Volumetric and isochoric part of the deformation:

$$\mathbf{C}_{\text{vol}} = (\det \mathbf{C})^{\frac{1}{3}} \mathbf{I}, \quad \bar{\mathbf{C}} = (\det \mathbf{C})^{-\frac{1}{3}} \mathbf{C}, \quad \mathbf{C} = \mathbf{F}^T \mathbf{F} \quad (3)$$

Decomposition of stress:

$$\mathbf{S} = S_{\text{vol}} \mathbf{C}^{-1} + \mathbf{S}_{\infty}^{\text{DEV}} + \mathbf{S}_{\text{ov}}^{\text{DEV}} \iff \mathbf{T} = \mathbf{F} \mathbf{S} \mathbf{F}^T = T_{\text{vol}} \mathbf{I} + \mathbf{T}_{\infty}^{\text{dev}} + \mathbf{T}_{\text{ov}}^{\text{dev}} \quad (4)$$

Material deviatoric operation:

$$\mathbf{S}^{\text{DEV}} = \mathbb{N}[\mathbf{S}] \quad \text{with} \quad \mathbb{N} := \left(\mathbb{I} - \frac{1}{3} \mathbf{C}^{-1} \otimes \mathbf{C} \right) \quad (5)$$

Classical deviatoric operation:

$$\mathbf{T}^{\text{dev}} = \mathbb{D}[\mathbf{T}] \quad \text{with} \quad \mathbb{D} := \left(\mathbb{I} - \frac{1}{3} \mathbf{I} \otimes \mathbf{I} \right) \quad (6)$$

Elastic law for the volumetric stress contribution:

$$S_{\text{vol}} = K (\det \mathbf{C})^{-\frac{1}{3}} \ln \left\{ \sqrt{\det \mathbf{C}} \right\} \quad (7)$$

Overstress of the Maxwell model:

$$\mathbf{S}_{\text{ov}}^{\text{DEV}} = 2G_{\text{ov}} (\det \mathbf{C})^{-\frac{1}{3}} \mathbb{N}[\mathbf{P}_V (\bar{\mathbf{C}}_{\text{ev}} - \mathbf{I}) \mathbf{P}_V^T] \quad \text{with} \quad \bar{\mathbf{C}}_{\text{ev}} = \mathbf{P}_V^T \bar{\mathbf{C}} \mathbf{P}_V \quad (8)$$

Equilibrium stress of the endochronic model:

$$\mathbf{S}_{\infty}^{\text{DEV}} = 2G_{\infty} (\det \mathbf{C})^{-\frac{1}{3}} \mathbb{N} \left[\mathbf{P}_P \left(\sum_{i=1}^3 s_i \mathbf{n}_i \otimes \mathbf{n}_i \right) \mathbf{P}_P^T \right] \quad \text{with} \quad \bar{\mathbf{C}}_{\text{ep}} = \mathbf{P}_P^T \bar{\mathbf{C}} \mathbf{P}_P, \quad (9)$$

$$s_i = \ln(1 + B(\lambda_i)) - (1 + D) \ln(1 - B(-\lambda_i)), \quad (\lambda_i, \mathbf{n}_i) = \text{Eigensystem}[\bar{\mathbf{C}}_{\text{ep}} - \mathbf{I}] \quad (10)$$

Evolution equation for the viscous transformation:

$$\dot{\mathbf{P}}_V \mathbf{P}_V^{-1} = -\frac{3}{2\eta} \left[\sinh \left(\frac{\sigma_{VV}}{\sigma_0} \right) \right]^k \frac{(\mathbf{S}_{\text{ov}}^{\text{DEV}} \mathbf{C})}{\sigma_{VV}} \quad (11)$$

Equivalent material overstress:

$$\sigma_{VV} = \sigma_{VV}(\mathbf{S}_{\text{ov}}^{\text{DEV}} \mathbf{C}) := \sqrt{\frac{3}{2} \text{tr}\{(\mathbf{S}_{\text{ov}}^{\text{DEV}} \mathbf{C})(\mathbf{S}_{\text{ov}}^{\text{DEV}} \mathbf{C})\}} \quad (12)$$

Evolution equation for the plastic transformation:

$$\dot{\mathbf{P}}_P \mathbf{P}_P^{-1} = -\frac{3}{2} \left(\frac{w_t}{Y} + \frac{w_c}{Y(1+D)} \right) \sigma_{VP} \dot{\varepsilon}_V \frac{(\mathbf{S}_{\infty}^{\text{DEV}} \mathbf{C})}{\sigma_{VP}} \quad (13)$$

Equivalent material equilibrium stress:

$$\sigma_{VP} = \sigma_{VP}(\mathbf{S}_{\infty}^{\text{DEV}} \mathbf{C}) := \sqrt{\frac{3}{2} \text{tr}\{(\mathbf{S}_{\infty}^{\text{DEV}} \mathbf{C})(\mathbf{S}_{\infty}^{\text{DEV}} \mathbf{C})\}} \quad (14)$$

Equivalent strain rate:

$$\dot{\varepsilon}_V := \sqrt{\frac{2}{3} \text{tr}\{\mathbf{D}^{\text{DEV}} \mathbf{D}^{\text{DEV}}\}} \quad (15)$$

Table 1 (continued)

Volumetric and isochoric part of the deformation:

Stress mode concentration factors:

$$w_i = \frac{1}{2}(1 + \xi), \quad w_c = \frac{1}{2}(1 - \xi) \quad \text{with} \quad \xi := \frac{\sqrt{27}}{2} \frac{J_3}{(J_2)^{3/2}} \quad \text{and} \quad J_i := \frac{1}{i} \text{tr}[(\mathbf{S}^{\text{DEV}} \mathbf{C})^i] \quad (16)$$

Permanent and non-permanent SDE-hardening evolution equations:

$$\dot{D} = \dot{D}_p + \dot{D}_n \quad (17)$$

$$\dot{D}_p = K_1 w_c \sigma_{VP} \dot{\epsilon}_V (D_p^{\text{max}} - D_p) \quad (18)$$

$$\dot{D}_n = K_2 w_c \sigma_{VP} \dot{\epsilon}_V (D_n^{\text{max}} - D_n) - w_c K_3 (D_n)^{K_4} \quad (19)$$

Table 2

Model parameters identified for filled PTFE

$K [\frac{\text{N}}{\text{mm}^2}]$	$G_{\infty} [\frac{\text{N}}{\text{mm}^2}]$	B	$G_{\text{ov}} [\frac{\text{N}}{\text{mm}^2}]$	$Y [\frac{\text{N}}{\text{mm}^2}]$	$\eta [\text{s}^{-1}]$	κ	$\sigma_0 [\frac{\text{N}}{\text{mm}^2}]$
3020.8	0.43	380.0	85.6	9.0	9×10^5	2.2	1.2
$K_1 [1/\text{s}]$	$K_2 [1/\text{s}]$	$K_3 [1/\text{s}]$	K_4	D_p^{max}	D_n^{max}		
10.0	50.0	0.5×10^{-4}	2.5	1.25	1.5		

(LINK1). The Coulomb-type frictional contact between the seal and the shaft has been described by point-to-surface contact elements (CONTACT48).

Fig. 2 illustrates the mounting process and the development of the radial displacements of the seal. While the shaft is moving from right to left through the clamped sealing element, the seal is strained (circumferential direction) and bent (radial direction).

The final distribution of logarithmic hoop strains, equivalent Huber-von-Mises stresses and volumetric stresses are also documented in Fig. 2. The hoop strains increase (nearly linear) towards the lip end. The maximum of the equivalent Huber-von-Mises stresses in the seal lip can be found in the regions of the highest hoop strains. Compressed regions can be found on the upper side of the seal whereas the elongated parts are on the lower side.

The time dependent reduction of the contact pressure along the contact zone of the seal and the shaft is shown in Fig. 3(a). Due to the asymmetric pressure distribution, the decrease of pres-

sure is different for different contact points. A common proportional factor between the time dependent reduction of the “radial force” F_R (integrated pressure, see Fig. 3(b)) and the contact pressure does not exist.

The relaxation process of the calculated radial force is shown in Fig. 3(b), together with the measured curves. The experimental setup is described in detail in Pohl [14]. The agreement between the experimental data and the calculated values is satisfactory, if the SDE is taken into account. The neglect of the SDE in the numerical simulation of PTFE shaft seals made of glass fibre filled compounds cannot be successful as illustrated by Fig. 3(b).

4. Final conclusions

A finite endochronic viscoplastic material model based on material isomorphisms is presented. An endochronic flow rule is applied to model the equilibrium hysteresis of the investigated PTFE

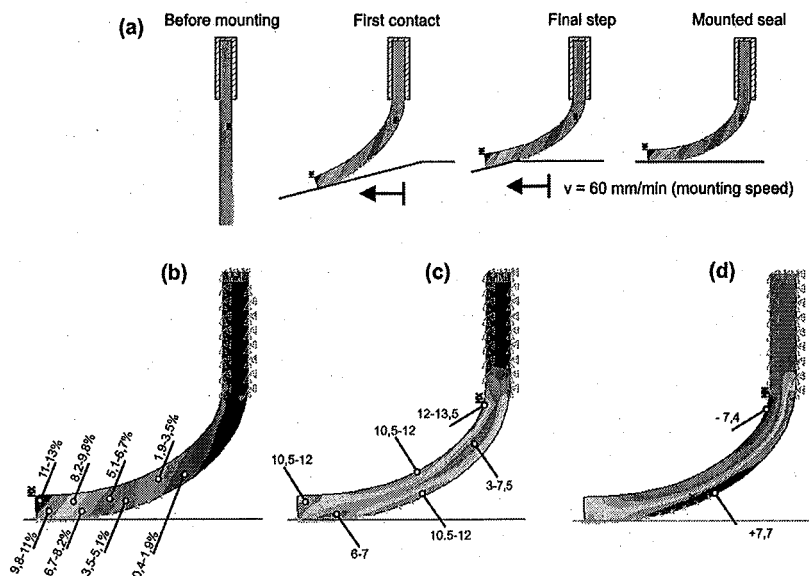


Fig. 2. Distribution of stresses and strains in a mounted seal. (a) Mounting process of a PTFE shaft seal, (b) Hoop strain, (c) Huber-von-Mises stress (N/mm²), (d) volumetric stress (N/mm²).

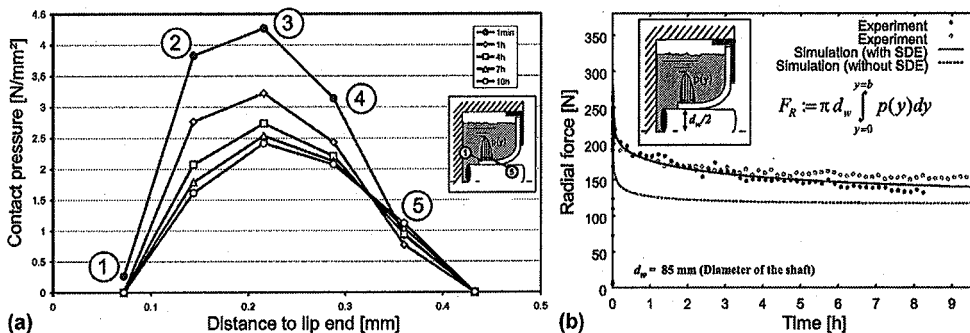


Fig. 3. Contact pressure and radial force. (a) Relaxation of the contact pressure, (b) relaxation of the radial force F_R .

compound, and a rate-dependent flow rule of the Garofalo-type is used to describe its time-dependent properties. Each inelastic flow rule is well known by itself. A new approach is their successful combination in a unified viscoplastic material model of the overstress type. In addition, in order to model the nonlinearities during active loading as well as during unloading, a nonlinear elastic law is applied to model the equilibrium stress. This approach allows to describe common inelastic phenomena (stress relaxation, strain rate dependence, plastic deformation, creep) and special effects

(SDE) in the mechanical behaviour of thermoplastic materials. The model has been identified for filled PTFE and numerical simulations of PTFE shaft seals have been performed using the finite element method. The results of these simulations are in fair agreement with the experimental data. Future work will be focused on numerical simulations of PTFE shaft seals with respect to the temperature dependence, inspired by the procedure described in Garofalo [6], and the dependence of the model parameters on the glass fibre volume fraction.

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