Mechanical modeling of rheometer experiments: Applications to rubber and actin networks

Michael J. Unterberger, Hannah Weisbecker, Gerhard A. Holzapfel*

Institute of Biomechanics, Graz University of Technology, Kronengasse 5-4, 8010 Graz, Austria

1. Introduction

Rotational rheology with a parallel-plate geometry is the state-of-the-art experimental method for the mechanical characterization of materials such as (cross-linked) actin networks. The deformation of the samples in such experiments resembles the torsion of a cylinder. In several previous studies, however, simple shear was used as an approximation for the real situation in parallel-plate rheometry, see, e.g., [1–3]. One aim of the present study is to analyze and quantify this commonly used approximation.

During experiments with a parallel-plate rheometer and plate radius \( R \) the axial force \( \tilde{N} \) and the applied torsion couple \( \tilde{M}_t \) are recorded and transformed into a normal stress component \( \tilde{\sigma} \) and a shear stress component \( \tilde{\tau} \), respectively. Thus [4],

\[
\tilde{\sigma} = \frac{\tilde{N}}{\pi R}, \quad \tilde{\tau} = \frac{2\tilde{M}_t}{\pi R^2}
\]

where the superimposed tilde is used to identify the values obtained from experimental tests.

Torsion of a cylinder undergoing large deformations in the context of rubber elasticity was solved in the seminal paper series of the single filament model [1–3,13,14]. This approach models the properties of a single actin filament first to obtain a force–stretch relationship. Based on that, a network model is then employed to homogenize the discrete microstructure. In our study the parameters of the resulting continuum mechanical constitutive model are interpretable as the properties of the single filaments and the network topology.

In the present study, we show that simple shear may be used for certain types of material models to investigate the torsional response. Furthermore, we show that by using an affine network model for capturing the mechanical response of cross-linked actin networks, we obtain a tensile normal stress (also for the simple shear case) which is in accordance with, e.g., [14]. On the other
hand, the eight-chain model is not able to generate tensile normal stresses. Subsequently, we distinguish three types of notation: (i) the tilde (\(\tilde{\cdot}\)) indicates rheological experiments with its measures as in (1), (ii) the hat (\(\hat{\cdot}\)) characterizes values which are related to simple shear, while (iii) no specific symbol refers to the torsion of a cylinder.

Section 2 establishes the governing equations for the torsion of a cylinder and conducts a comparison to simple shear. Subsequently, in Section 3, we apply the findings to material models for rubber and deformation in Section 4 we focus on models for cross-linked actin networks. Specifically, we investigate an eight-chain model and an affine constitutive model for cross-linked F-actin networks. In the final Section 5, we provide a discussion and conclude the study.

2. Analytical solution of the torsion of a cylinder

In this section we briefly review the necessary kinematics required for the analysis of the torsion of a cylinder at finite strains. We introduce the most general form of the stress relation together with simple shear as a local approximation of simple torsion. Subsequently, we specialize these relations to materials which can be described in terms of strain invariants.

2.1. Non-linear continuum mechanics

Consider an incompressible circular cylinder with radius \(R\) and height \(Z\) in cylindrical polar coordinates \((r, \phi, z)\), as depicted in Fig. 1. A point in the reference and the current configuration are characterized by the position vectors \(\mathbf{X}\) and \(\mathbf{x}\), respectively. The index zero is employed to note the coordinates in the reference configuration, i.e. \((r_0, \phi_0, z_0)\). Hence, we describe the deformation through

\[
\mathbf{F} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & k \rho \\ 0 & 0 & 1 \end{bmatrix},
\]

where \(k\) is the twist, with the unit \(1\text{ m}^{-1}\). The angle \(\phi\) by which the top surface is rotated with respect to the bottom surface is \(\phi = kZ\). Hence, the deformation gradient \(\mathbf{F}\) is given in the matrix form as

Fig. 1. Cylinder under torsion (dimensions \(R\) and \(Z\)) with a cylindrical coordinate system \((r, \phi, z)\). The components of the tangent vector \(\mathbf{dx}\) associated with the position vector \(\mathbf{x}\) are \(\mathbf{dx} = \mathbf{dr}\) and \(d\phi\) and \(dz\). The dash-dotted lines on the cylinder in the reference configuration deform to the dotted lines in the current configuration. The angle of rotation is \(\phi = kZ\), defined through the twist \(k\). The gray areas schematically represent the distributions of shear stress \(\sigma_{ss}\) and normal stress \(\sigma_{zz}\) over the radius \(r\).

representing the linear transformation of a tangent vector \(d\mathbf{X}\) in the reference configuration to the current configuration \(d\mathbf{x}\), i.e. \(d\mathbf{x} = \mathbf{F} d\mathbf{X}\). The first invariant \(I_1 = \text{tr} \mathbf{C}\) of the right Cauchy–Green tensor \(\mathbf{C} = \mathbf{F}^T \mathbf{F}\) is

\[
I_1 = k^2 r^2 + 3.
\]

Note that \(J = \det \mathbf{F} = 1\), characterizing a volume-preserving deformation.

Assume now that the constitutive relation of the material can be expressed by the strain–energy function \(\Psi(\mathbf{C})\) in terms of the right Cauchy–Green tensor. The Cauchy stress tensor \(\mathbf{\sigma}\) is then given as

\[
\mathbf{\sigma} = \mathbf{\sigma} - p \mathbf{I},
\]

(5)

where \(\mathbf{\sigma} = 2\mathbf{F} \partial \Psi / \partial \mathbf{C}^T \mathbf{F}\) and \(p\) is a Lagrange multiplier associated with the incompressibility constraint which can be interpreted as a hydrostatic pressure. Assuming a static problem and neglecting body forces, the key equation is then the equilibrium in the radial direction, i.e.

\[
d\sigma_{rr} + \frac{1}{r}(\sigma_{rr} - \sigma_{\phi\phi}) = 0.
\]

The equations for the circumferential and the axial directions lead to the conclusion that \(p\) does not change through the sample thickness or in the circumferential direction, but only in the radial direction. The radial normal stress \(\sigma_{rr}\) on the side surface of the cylinder must vanish, leading to the boundary condition

\[
\sigma_{rr}|_{r = R} = 0.
\]

Then, by using (5) in (6) and subsequent integration we obtain

\[
p = \sigma_{rr} + \int_{r}^{R} \frac{(\sigma_{rr} - \sigma_{\phi\phi}) dr}{r^2}
\]

for the hydrostatic pressure. This equation combines the equilibrium equation with the boundary condition, and hence all components of (5) are determined.

When conducting an experiment, as illustrated in Fig. 1, we rotate the top plate with respect to the bottom one by an angle \(\phi\) while holding the distance \(Z\) between the plates constant. Simultaneously we measure the torsion couple \(M_t\) applied to the sample and the required axial force \(N\) to keep the distance between the plates constant. The axial force \(N\) is simply given by

\[
N = \int_A \sigma_{zz} dA,
\]

where \(A\) is the top surface of the cylinder. The torsion couple \(M_t\) is obtained by integration of the shear stress, which is the force per deformed area, multiplied by the lever \(r\), i.e.

\[
M_t = \int_A \sigma_{\phi\phi} dA.
\]

Note that for the cylinder \(dA = r \ dr \ d\phi\), with \(\phi \in [0, 2\pi]\) and \(r \in [0, R]\). A conversion to the equivalent stress components, analogous to (1), may be applied. Thus

\[
\frac{\sigma}{\pi R^2} = \frac{2M_t}{\pi R^2}
\]

are the related normal stress and shear stress components, respectively.

2.2. Simple shear as a local approximation

Simple shear may be seen as a local approximation of simple torsion of a circular cylinder since the torsion deformation of the 3D surface of a cylinder can be reduced to a plane simple shear deformation in the local neighborhood of a point. More precisely, it is the solution at the outer surface \(r = R\) of the cylinder.
The curvilinear coordinates \((r, \phi, z)\) correspond to the Cartesian coordinates \((x, y, z)\). The non-trivial component of the deformation gradient \((3)\) is commonly abbreviated by \(\gamma = kR\). According to \((5)\) the radial stress component reads \(\sigma_{rr} = -\pi_{rr} - p\) so that the hydrostatic pressure can explicitly be expressed as \(p = \pi_{rr} \big| r = R\) by using the boundary condition \((7)\). Hence, the non-zero components of the Cauchy stress tensor are then
\[
\sigma_{yy} = \pi_{\phi\phi} \big| r = R - \pi_{rr} \big| r = R, \quad \sigma_{zz} = \pi_{zz} \big| r = R - \pi_{rr} \big| r = R, \quad \sigma_{yz} = \pi_{\phi z} \big| r = R.
\]

Let us now compare \((12)_1\) with the result of a hypothetical experiment by combining \((11)\) with \((10)\), i.e.
\[
\tau = 4 R I_1 \int_0^R r^2 \sigma_{\phi z}(r) \, dr.
\]
Equivalence between the two equations is then achieved, when \(\sigma_{\phi z}(r)\) is linear in \(r\). More precisely, when \(\sigma_{\phi z}(r) = K \gamma r / R\), where \(K\) is a constant, then \(\tau = \sigma_{yz} = K \gamma\). Unfortunately, there does not exist a closed form relationship for the comparison of the normal components \(\sigma\) and \(\sigma_{zz}\).

2.3. Specialization of the material model

Assume now an isotropic material from which we can express the strain–energy function \(\psi(l_1, l_2)\) in terms of the first and second invariants \((l_1, l_2)\) of the left Cauchy–Green tensor \(b = FF^\top\). The third invariant \(I_3 = J^3\) constitutes the kinematic constraint of incompressibility. Note that these invariants are identical to those of the right Cauchy–Green tensor \(C\). Then, the first term in \((5)\) is
\[
\Pi = 2\psi \big| b - 2\psi \big| b^{-1},
\]
where \(\psi_i = \partial \psi / \partial l_i, i = 1, 2\). Using the components \(\pi_{rr}, \pi_{\phi\phi}\) and \(\pi_{\phi z}\) of \((14)\) in \((8)\), the non-zero Cauchy stress components are then given according to \((5)\) in the closed forms
\[
\sigma_{rr}(r) = 2 \psi_1 k^2 r^2 + 2 k^2 \int_0^r \psi_1 r^* \, dr^*,
\]
\[
\sigma_{\phi\phi}(r) = 2 \psi_1 k^2 r^2 + 2 k^2 \int_0^r \psi_1 r^* \, dr^*,
\]
\[
\sigma_{zz}(r) = -2 \psi_2 k^2 r^2 + 2 k^2 \int_0^r \psi_1 r^* \, dr^*, \quad \sigma_{\phi z}(r) = 2 k \psi_1 \psi_2 r^2.
\]

The axial force \(N\) and the torsion couple \(M_t\) are calculated according to \((9)\) and \((10)\), respectively. Thus, with \((16)\) we obtain the explicit expressions in terms of \(\psi_1\) and \(\psi_2\), i.e.
\[
N = 4 \pi k \int_0^R \left( -\psi_2 r^2 + \int_0^r \psi_1 r^* \, dr^* \right) r \, dr,
\]
\[
M_t = 4 \pi k \int_0^R (\psi_1 + \psi_2) r^3 \, dr,
\]
for the results \((15)\)–\((17)\) see also \([16]\). Using \((17)\) in \((11)\) allows a similar comparison as in the previous section. The general arguments made therein may be specialized and from \((15)\) and \((16)\) we obtain the non-zero Cauchy stress components for simple shear, i.e.
\[
\sigma_{yy} = 2 \psi_1 r^2, \quad \sigma_{zz} = -2 \psi_2 r^2, \quad \sigma_{yz} = 2 (\psi_1 + \psi_2) r^2.
\]
We conclude that \(K = 2 (\psi_1 + \psi_2)\) must be a constant to obtain equivalent shear stress results for the torsion of a circular cylinder \(r\) and simple shear \(\sigma_{yz}\). On the other hand, the normal stress calculated from \((17)\) in \((11)\) shows that the solution for the torsion of a cylinder \(\sigma(\psi_1, \psi_2)\) depends on the derivatives of the strain–energy function with respect to both invariants while the simple shear solution \(\sigma_{yz}\) depends only on the derivative with respect to the second invariant \(I_2\). Thus, an equality between the two measures would require a material model which is only dependent on \(I_2\).

Truesdell and Noll [6] pointed out that Eqs. \((15)\), \((16)\) and \((18)\) use the same coefficients \(\psi_1\) and \(\psi_2\), which, in general, depend on \(k\) and \(r\). It is, therefore, possible to measure the shear and one normal stress component and from that calculate the behavior of a cylinder subject to torsion.

3. Solutions for some isotropic constitutive rubber models

For subsequent analyses consider now three different material models. The Mooney–Rivlin model and its specialization, i.e. the neo-Hookean model, are very frequently used in rubber elasticity. Thereby, the shear modulus is constant. Finally, we use the Yeoh model as a representable model for a variable shear modulus.

The strain–energy function of the 2-parameter Mooney–Rivlin material is
\[
\psi_{MR} = c_1 (l_1 - 3) + c_2 (l_2 - 3),
\]
where \(c_1\) and \(c_2\) are positive material constants. Hence, Eqs. \((16)\) and \((17)\) simplify to
\[
\sigma_{yz}^{MR} = -c_1 k^2 (R^2 - r^2) - 2 c_2 k^2 r^2, \quad N_{MR} = -\pi k^2 R^4 \left( c_1 / 2 + c_2 \right).
\]

For convenience, we introduce the shear modulus \(\mu\) according to \(\mu = 2 (c_1 + c_2)\),
\[
\sigma_{yz}^{NH} = \frac{\mu}{2} (l_1 - 3),
\]
where we require \(c_1 + c_2 > 0\) in order to achieve a physically correct behavior. Hence, for a neo-Hookean model of the form
\[
\psi^{NH} = \frac{\mu}{2} l_1 - \frac{3\mu}{4} k^2 R^4,
\]
(23)

These results can also be found in the literature, see, e.g., [4, 16] or the extensive work of Rivlin [17–20], with different approaches selected for the derivation. The negative sign of the axial force was confirmed experimentally by Rivlin and Saunders [20], following experiments on wires performed by Poynting [21].

By evaluating \((16)_2\) and \((17)_2\), the shear stress and the torsion couple are given by
\[
\sigma_{yz}^{MR} = \frac{\sigma_{yz}^{NH}}{k} = \mu k r, \quad M_t^{MR} = \frac{M_t^{NH}}{k^2} = \pi k^4 R^4 / 2,
\]
respectively. These expressions hold for both material models, where \(\mu\) is defined in \((21)\). Note the (very) high sensitivity of the torsion couple in \((24)_2\) to changes in the radius \(R\).

Fig. 2 shows the Cauchy shear stress \(\sigma_{yz}\) and the normal stress \(\sigma_{zz}\) as a function of the radius \(r\) for the neo-Hookean and Mooney–Rivlin models. The radius of the cylinder is \(R = 25\) mm and the twist is \(k = 8 \text{ m}^{-1}\). Both material models possess a shear modulus of \(\mu = 1 \text{ MPa}\) while the Mooney–Rivlin model uses the additional relation \(c_1 = 7 c_2\) [20]. The relationship of the shear stress \(\sigma_{yz}\) and the radius \(r\) is linear, see \((24)_1\), and both models provide the same result. The normal stress \(\sigma_{zz}^{NH}\) for the neo-Hookean model, see Fig. 2(a), is compressive (denoted by a negative sign) with the largest magnitude at the center of the disc. It vanishes at the outer surface in contrast to the normal stress \(\sigma_{zz}^{MR}\) for the Mooney–Rivlin model, see Fig. 2(b), which shows a finite compressive stress at the outer surface.

The Yeoh model [7] with the strain–energy function \(\psi_{YEH}^{\text{YEOH}}\) is an example for a constitutive equation with a variable shear stiffness given as
\[
\psi_{YEOH} = d_1 (l_1 - 3) + d_2 (l_1 - 3)^2 + d_3 (l_1 - 3)^3,
\]
with the three material constants \(d_1 > 0, d_2 < 0, d_3 > 0\). With this model, Eqs. \((16)\) and \((17)\) give the normal stress \(\sigma_{zz}^{YEOH}\) and the
The shear stress \( \tau \) in the direction of the simple shear solution characterized by the amount of shear \( \gamma \), is higher than the simple shear approximation for the Yeoh model and the Mooney-Rivlin model, \( \mu = 1 \) MPa, \( c_1 = 1/2c_2 \) (b) and the Yeoh model, \( d_1 = 0.5 \) MPa, \( d_2 = -d_1/2, d_3 = d_1/6 \) (c). The stress values at the outer radius \( R \), marked by circles, do correspond to the simple shear solution characterized by the amount of shear \( \gamma = k \delta R = 0.2 \), with \( R = 25 \) mm (compare with Section 3). Note that the Mooney-Rivlin model predicts a non-zero normal stress at the outer radius and the shear stress response for the neo-Hookean and Mooney-Rivlin models is the same.

The material parameters remain those introduced in the previous approximation for the Yeoh model and the Mooney-Rivlin model, \( \mu = 1 \) MPa, \( c_1 = 1/2c_2 \) (b) and the Yeoh model, \( d_1 = 0.5 \) MPa, \( d_2 = -d_1/2, d_3 = d_1/6 \) (c). The stress values at the outer radius \( R \), marked by circles, do correspond to the simple shear solution characterized by the amount of shear \( \gamma = k \delta R = 0.2 \), with \( R = 25 \) mm (compare with Section 3). Note that the Mooney-Rivlin model predicts a non-zero normal stress at the outer radius and the shear stress response for the neo-Hookean and Mooney-Rivlin models is the same.

The error for the models with linear shear elasticity is zero. The error for the models with linear shear elasticity is zero. The error for the models with linear shear elasticity is zero. The error for the models with linear shear elasticity is zero.

The shear stress \( \sigma_{yy}^{YEOH} \) and the torsion couple \( M_t^{YEOH} \) are calculated from (16) and (17), i.e.

\[
\sigma_{yy}^{YEOH} = 2kr(d_1 + 2dkD^2 + 3dkD^4),
\]

\[
M_t^{YEOH} = ekR^4 \left(d_1 + \frac{4}{3}dkD^2 + \frac{4}{3}dkD^4 \right).
\]

The relationships between the Cauchy stress components, i.e. \( \sigma_{yy}^{YEOH} \) and \( \sigma_{zz}^{YEOH} \), and the radius \( r \) are depicted in Fig. 2(c), where the parameters are \( d_1 = 0.5 \) MPa, \( d_2 = -d_1/2 \) and \( d_3 = d_1/6 \). The behavior is very similar to the neo-Hookean model. The non-linear terms in (25), however, generate a convex curve for the shear stress. Further analysis of the Yeoh model is presented in the subsequent section. It is important to note that the shear stress response for the neo-Hookean and Mooney-Rivlin models is the same.

For all introduced models closed-form solutions for the axial force \( N \) and the torsion couple \( M_t \), resulting from the deformation characterized through (3), can be obtained. We may therefore compare those values to the respective quantities \( N \) and \( M_t \), measured in experiments, as it was done by Rivlin and Saunders [20]. The calculation of the stress measures (1) is, hence, not necessary for parameter identification.

We can also solve the torsion of a circular cylinder by means of the finite element method.

### 3.1. Error measures for the torsion couple and the axial force

Recall that (11) gives the exact answer only if \( \sigma_{xx} \) depends linearly on \( r \). Hence, when we use (11) for the Yeoh model, it denotes a value for the shear stress \( \tau^{YEOH} \) which does not coincide with the simple shear solution, see Fig. 3(a). This observation may be generalized for all material models where \( \psi_1 \) or \( \psi_2 \) are dependent on \( r \). Fig. 3 compares the results of a hypothetical experiment, where the torsion couple and the axial force of Section 2 are evaluated according to (11) to the simple shear approximation for the Yeoh model and the Mooney–Rivlin model. The material parameters remain those introduced in the previous section. The shear stress \( \tau^{YEOH} \) for the non-linear Yeoh model, Fig. 3 (a), is higher than the simple shear approximation \( \tau^{YEOH} \), while the shear stresses \( \tau^{MR} \) and \( \tau^{YEOH} \) for the Mooney-Rivlin model with its constant shear modulus, Fig. 3(b), coincide. Recall, that for simple shear \( \tau^{YEOH} = 0 \) because \( \psi_2 = 0 \), see (18) and [22,23]. Considering, for example, the Yeoh model, Fig. 3(a), the value \( \tau^{YEOH} \) of the normal stress is zero over the whole range of \( r \). On the other hand, the average normal stress \( \sigma \) calculated from (11) implies the compressive force, as discussed in Section 2. For the Mooney–Rivlin material, Fig. 3(b), where \( \psi_2 = c_2 \) we obtain the correct tendency of the normal stress \( \sigma^{YEOH} \) behavior. The curves, however, do not coincide.

Assuming that we approximate the shear stress data of a hypothetical experiment using Eq. (18) for simple shear. Then, by identifying \( \sigma_{xx} \) with \( r \) in (11) we obtain an estimated (approximate) torsion couple of \( M_t = \psi_1(r) + \psi_2(r)R^3 \). This expression only recovers the torsion couple calculated from (10) for a constant shear modulus. For non-linear models, however, a discrepancy between the estimated torsion couple and the real (theoretical) torsion couple becomes apparent. For example, for the Yeoh model, by using the relations \( \gamma = Rk \) and \( l_1 = R^2 + 3 \), the error is calculated as a percentage difference between \( M_t \) and \( M_t^{YEOH} \), i.e.

\[
e_{NN} = \left| \frac{M_t^{YEOH} - M_t^{YEOH}}{M_t^{YEOH}} \right| = \frac{2d_3\gamma^2/3 + 3d_3\gamma^4/2}{d_1 + 4d_3R^2/3 + 3d_3R^4/2}.
\]

With our material parameter values, at \( \gamma = 0.5 \), we obtain \( e_{NN} = 8\% \). The error for the models with linear shear elasticity is zero.

For the quantification of the axial force error we may define a measure analogous to (30). For the Mooney–Rivlin material we obtain

\[
e_{NN} = \left| \frac{M_t^{MR} - M_t^{MR}}{M_t^{MR}} \right| = \frac{2c_2 - c_1}{c_1 + 2c_2}.
\]

In this case, the error is independent of the amount of shear. The error is \( e_{NN} = 56\% \) with the previous parameters.

### 4. Implications to continuum models for cross-linked actin networks

In this section we apply the findings of Section 2 to network models, in particular to the eight-chain model [24] originally developed for rubber elasticity and to a recently proposed affine constitutive model for cross-linked actin networks [13]. Differences between the torsional and the simple shear solutions are highlighted for these network models. Since these types of network models are able to use any filament model, described by a strain–energy function, the choice for a specific filament model is of minor importance. We are here primarily interested in the
effect of the network models on the mechanical response and, therefore, we use one filament model for both networks to adequately visualize their difference.

Consider an actin filament for which we desire to use a relationship between the stretch \( \lambda \) and the tensile force \( f \) of the form [3,25]

\[
\frac{r_0}{L} = 1 + a^{f^*} - \left( 1 + a^{f^*} \right)^{1/2} \left( 1 - r_0/L \right),
\]

(32)

where we have used the shorthand notation \( a = \kappa^2 k_b T \rho / (\mu_0 L^2) \) and the dimensionless force \( f^* = f L^2 / (\kappa^2 k_b T \rho) \) with the parameters: Boltzmann constant \( k_b \), temperature \( T \), persistence length \( L_p \), stretch modulus \( \mu_0 \) and contour length \( L \) of the filament. In addition, we have used the relative extensional number \( \delta \) and the end-to-end distance \( r_0 \) at zero force (note that \( r_0 \) is not identical to the reference radius introduced in (2)). We require that the filaments bear only tensile loads and set \( f = 0 \) for the case that \( \lambda \leq 1 \). The free energy \( w(\lambda) \) of the single filament is the integral of the tensile force \( f \) along the end-to-end distance \( r = r_0 \) (with \( r \) not to be confused with the current radius in (2)). The derivative of the filament strain energy with respect to the stretch \( \lambda \) is, by the chain rule [3],

\[
w' = f r_0,
\]

(33)

i.e. a function of the tensile force which is defined in (32).

4.1. Eight-chain model

The eight-chain model [24] was recently combined with the chain model by MacKintosh et al. [26] and applied to actin networks [2]. This network model considers a representative volume element containing eight polymer chains which are attached to each other at the center of the cube. The other ends of the filaments are connected to the vertices of the cube. Instead of the model of MacKintosh et al. [26] we now use (32) and define the total chain stretch as

\[
\lambda = \lambda_0 \lambda_{AB},
\]

(34)

where \( \lambda_0 \) is a pre-stretch required to achieve a non-zero initial shear modulus, and

\[
\lambda_{AB} = \sqrt{1/3} = \sqrt{(k^2 r^2 + 3)/3}
\]

(35)

is the homogenized chain stretch obtained from the eight-chain model [24], where the explicit expression [4] for the first invariant has been used. With the filament density \( n \) the strain-energy function \( \psi_{AB} \) for the filament network is \( n w \). Then, with the chain rule and the properties (34) and (35) we get

\[
\psi_1 = \frac{n l_0}{B} w', \quad \psi_2 = 0.
\]

(36)

We then use these two relations in (16) to obtain \( \sigma_{AB}^{\text{MR}} \) and \( \sigma_{i}^{\text{AB}} \) by means of numerical integration. Consequently, from (17) we are able to calculate the axial force \( N_{AB} \) and the torsion couple \( M_{AB} \).

By analogy with Figs. 2 and 3 we illustrate the plots for the eight-chain model in Fig. 4(a) and (c). The material parameters we used are end-to-end distance at zero force \( r_0 = 1.63 \mu m \) [13,27], persistence length \( L_p = 16 \mu m \) [28], relative extensional number \( \delta = 0.5 \) [13], filament density \( n = 8.57 \mu m^{-3} \), contour length \( L = 1.78 \mu m \) and stretch modulus \( \mu_0 = 117.5 \mu N \); an explanation for the parameters \( n, L \) and \( \mu_0 \) is provided in the next section. For comparison purposes we give the eight-chain model an initial shear modulus by choosing a slight pre-stretch (\( \lambda_0 = 1.001 \)). The shear stress \( \sigma_{AB}^{\text{MR}} \) increases non-linearly over the radius \( r \), while the normal stress \( \sigma_{i}^{\text{AB}} \) shows a similar characteristics as for the neo-Hookean model (compare with Fig. 2(a)). Again, the simple shear solution is recovered at \( r = R \), indicated by the circle. In Fig. 4(c), the simple shear solution for the shear stress \( \sigma_{i}^{\text{MR}} \) overestimates the result for the isotropic network. In analogy to (30), the error at \( r = 0.2 \) is \( \epsilon_{MN}^{\text{MR}} = 44\% \). Recall that the strain–energy function of the eight-chain model is only dependent on the first invariant \( I_1 \) of the right Cauchy–Green tensor, and thus the simple shear solution predicts a zero normal stress \( \sigma_{i}^{\text{AB}} \) according to (18) [2] and [23]. The torsion of the cylinder gives again a negative normal stress. This behavior is similar to the neo-Hookean and Yeoh models.

4.2. Affine constitutive model for cross-linked F-actin networks

We consider an affine constitutive model and introduce an actin filament whose orientation is described by the unit vector \( \mathbf{m} \) with respect to the reference configuration. Applying the deformation gradient \( \mathbf{F} \) on \( \mathbf{m} \) we obtain the deformed vector \( \mathbf{m} = \mathbf{F} \mathbf{m} \). The stretch of the filament is then given by the length of \( \mathbf{m} \), i.e. [15]

\[
\lambda = (\mathbf{m} \cdot \mathbf{m})^{1/2} = (\mathbf{M} \cdot \mathbf{C} \mathbf{M})^{1/2}.
\]

(37)

Based on the theory for affine networks [29–31], the strain–energy function for an isotropic network is defined as the total strain energy of the single filaments per unit reference volume, i.e. [13]

\[
\psi_{\text{AN}} = \int_{\Omega} w(\lambda) \, d\Omega,
\]

(38)

where the superscript \( \text{AN} \) stands for the affine network model.

The first part of the Cauchy stress tensor (5) for an isotropic filament distribution is calculated as

\[
\sigma_{\text{AN}} = \int_{\Omega} \frac{w'}{\lambda} \mathbf{m} \otimes \mathbf{m} \, d\Omega.
\]

(39)
Recall the definition (33) for the single filament contribution \( w' \).
By using \( \mathbf{F} \) from (3) the vectors \( \mathbf{M} \) and \( \mathbf{m} \) in spherical coordinates are (in matrix form)

\[
[M] = \begin{pmatrix}
\sin \theta \cos \phi \\
\sin \theta \sin \phi \\
\cos \theta
\end{pmatrix}, \quad [m] = [F][M]
\]

in the reference and the current configuration, respectively. According to (37), the filament stretch \( \lambda \) is then

\[
\lambda = [1 + kr(\sin \phi \sin 2\theta + kr \cos^2 \theta)]^{1/2}.
\]

By means of a numerical integration we can solve the integral in (39) and calculate the hydrostatic pressure (8). By noting that

\[
\int_A A(\phi, \theta) \, d\Omega = \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} A(\phi, \theta) \sin \theta \, d\theta \, d\phi,
\]

where \( A(\phi, \theta) \) is an arbitrary second-order tensor, we may obtain the Cauchy stress tensor \( \sigma^{AN} \) according to (5) which, eventually, allows the numerical evaluation of (9) and (10) to calculate the axial force \( N^{AN} \) and the torsion couple \( M^{AN} \). In the case of simple shear, we assume a plane stress state, i.e. \( \sigma^{AN}_{yy} = \sigma^{AN}_{yz} = \sigma^{AN}_{zz} = 0 \) and identify \( p = \sigma^{AN}_{xx} \) to obtain the shear and normal stress components \( \tau^{AN}_{xy}, \tau^{AN}_{xz}, \sigma^{AN}_{zz} \), respectively.

\begin{table}[h]
\centering
\begin{tabular}{|l|l|l|}
\hline
Experiment parameter & \( a \) & \( b \) \\
\hline
\hline
Simple shear & 1.77 & 44.2 & 1.75 & 24.9 \\
Torsion of a cylinder & 1.78 & 98.2 & 1.78 & 117.5 \\
Relative difference & 0.006 & 0.55 & 0.017 & 0.79 \\
\hline
\end{tabular}
\caption{Parameters of the affine network model fitted to two experiments from [3], i.e. the contour length \( L \) and the stretch modulus \( \mu \), for the plots shown in Fig. 5, in addition to the relative difference between the parameters for simple shear and torsion of a cylinder normalized with respect to the torsion of a cylinder.}
\end{table}

Fig. 4(b) illustrates the distributions of the Cauchy shear stress \( \sigma^{AN}_{xx}, \sigma^{AN}_{xy} \) and normal stress \( \sigma^{AN}_{yy}, \sigma^{AN}_{zz} \) versus the radius \( r \). By comparing the values of the shear and normal stresses with the corresponding values in Fig. 4(a) of the eight-chain model, we observe that the values are three orders of magnitude larger. The characteristic difference of the affine network model with the eight-chain model is the normal stress \( \sigma^{AN}_{zz} \) which changes its sign at \( r \sim 17 \text{ mm} \) and is positive at the outer surface of the cylinder. This results in a positive axial force \( N^{AN} \). The comparison of the simple shear solution with the hypothetical experiment is depicted in Fig. 4(d). Similar to the eight-chain model, for simple shear the shear stress \( \sigma^{AN}_{xy} \) overestimates the response \( \gamma^{AN} \) of the hypothetical experiment for the affine network model. The error \( e_{\gamma^{AN}}^{AN} = 42\% \) is smaller...
the shear stress \( \tau \). Hence, in this case, the boundary conditions for the torsion of a cylinder give the better fit compared to simple shear. The obtained parameters differ by 1.7% and 79% for \( L \) and \( \mu_0 \), respectively.

5. Discussion and conclusion

In this study we analyzed the torsion of a solid circular cylinder that occurs in a rotational parallel-plate rheometer, and we provided three illustrative examples for constitutive models used in rubber elasticity: neo-Hookean, Mooney-Rivlin, Yeoh. We compared these results with the solution for simple shear and defined quantitative measures for the errors which occur due to this approximation. Finally, we applied the method to two more complex models for cross-linked biopolymer networks, where the error due to the simple shear approximation is even more pronounced.

The torsion of a cylinder (with a parallel-plate geometry) is characterized by a shear deformation of \( kr \) which is dependent on the radius \( r \). This property leads to a non-homogeneous shear stress in the sample. A constant shear deformation over the radius can be achieved for materials with constant shear modulus and a cone-and-plate geometry of the measuring chamber. For such a test setup the discrepancies between the simple shear response and the torsion response in terms of the shear stress would be eliminated. The hydrostatic pressure (5), however, would still generate a normal stress varying with the radius. Therefore, single stress values cannot represent the complex stress state of samples in rotational rheometry. The definitions (1) can only serve as auxiliary quantities.

Stress measures calculated from experiments are convenient in the modeling and the parameter identification by approximating the real boundary conditions by simple shear. The torsion couple is correctly captured for models with constant shear moduli (neo-Hookean and Mooney-Rivlin models) while a varying shear modulus imposes can cause an error. We never observed an exact reproduction of the axial force through the simple shear approximation, however, simple shear can capture the correct trend for the axial force for some material models, e.g., Mooney–Rivlin, Models with a strain–energy function only dependent on \( I_1 \), e.g., neo-Hookean, Yeoh and eight-chain models, unfortunately, do an inaccurate prediction of the normal stress \( \sigma_{xx} \) in the simple shear mode, namely zero [23]. Considering two actin network models, the torsion solution for the eight-chain model predicts a negative axial force which is in contrast to experimental results. For the affine network model, however, we obtained good predictions, namely a positive normal stress for both boundary conditions.
suggests that the model is more suitable for cross-linked actin networks. The difference in the predicted axial force between simple shear and torsion of a cylinder is very large which makes a simple shear approximation inaccurate. Compared to the Yeoh model, the larger deviation of the shear stress from the linear behavior appears to impose also a larger difference for the estimation of the torsion couple for the actin network models (AB: 44%; AN: 42%).

Experimental data of cross-linked actin networks available from rotational rheometry have low reliability of the axial force response [3]. The fact that we were able to fit the model with simple shear boundary conditions must not lead to the conclusion that simple shear provides a good approximation for the mechanical response of a cylinder under torsional loading. By picking a different sample with essentially identical shear stress behavior we can obtain a reasonably good fit to the model with torsion boundary conditions. Therefore, the axial force data from experiments can only serve as a trend for the real behavior, while a reliable measurement can only be conducted for the shear component.

In this study we focussed on the quasi-static behavior of samples in rotational rheometry. This allowed us to confine our investigations within the relatively simple framework of elasticity. Throughout the present work we assumed that the mechanical response of a cylinder under torsional loading, as it occurs during a rotational rheometer test with a parallel-plate geometry, can be modeled as a torsional problem of a cylinder; this is also convincingly supported by experiments on Vulcanized rubbers [20]. In the case of cross-linked actin networks, however, we need to consider that these materials are soft gels so that the behavior may differ from that of a solid.

Simple shear, in general, is not a good approximation for the mechanical response of a (solid) circular cylinder under torsional loading. Only for isotropic materials with constant shear moduli, the torsion couple is represented adequately by simple shear. Certainly, stress measures are convenient for the comparison of different samples. When it comes to parameter identification, however, it is advised to make use of the measured quantities, i.e. axial force and torsion couple. The large variations in the measured axial force during experiments of cross-linked actin filaments also call for improved rheometer designs or a more reliable measuring technique.

References