

Constitutive models for the stress tensor based on nonaffine motion

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CONSTITUTIVE MODELS FOR THE STRESS TENSOR
BASED ON NONAFFINE MOTION

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INTRODUCTION

A rather general, but relatively simple framework for the description of differential type constitutive equations for the stress tensor for polymer melts and solutions is presented. The purpose of these equations is the use in numerical simulations of unsteady flows in complex geometries of polymer solutions and melts. Therefore, the final constitutive equations should be formulated without any molecular quantities, i.e. variables that represent aspects of the microstructure in its full detail. However, in building these equations it is important that some foundation in the microstructure and the evolution of it, is kept. At the same time also mathematical convenience is strived for. This leads to a semi-empirical approach which gives the opportunity to force the constitutive equations to be relatively simple and still flexible enough to fit the complex flow behaviour of polymer melts and solutions.

Many of the existing constitutive models, although based on detailed modeling of the microstructure and therefore sometimes very complex, do not satisfy; their predictive capacity is not sufficient. Examples are the bead-spring model with hydrodynamic interaction and the Doi/Edwards model. Besides, equations that are rigorous and more accurate are in general very complex and unwieldy. They are impracticable for numerical simulations of complex unsteady flows.

Therefore the following objects are set out in this study:

- Summarize existing models in the framework.
- To be able to describe the behaviour of polymer melts and solutions.
- Constitutive equations should be convenient for use in numerical simulations.
- Have a restrictive complexity in order to limit computer time.

STRUCTURAL ELEMENTS WITH A LINEAR SPRING BEHAVIOUR

The main parts of the modelling are:

- 1) An expression for the average stress tensor (the macroscopic Cauchy stress tensor)
- 2) A constitutive equation for the rate of change of the length of the relevant structural element on a microscopic level.

The structure of the material is modelled as a number of sets of particles, the relevant structural elements, which are represented by vectors \vec{R}_i . From the virtual work principle it follows that the contribution to the average stress tensor of particles of type i , the relevant structural element of type i , is given by:

$$\sigma_i = \zeta \nu \langle \vec{f}_i \vec{R}_i \rangle$$

where ν = number density (per unity of volume) of the particles, \vec{f}_i the force acting on a particle, \vec{R}_i the characteristic length of the particle and $\langle \cdot \rangle$ means the average over a non-equilibrium configuration distribution function ψ for the lengths \vec{R}_i (an average in the \vec{R} -space). The factor ζ is a force reducing factor without, yet, a physical meaning. It is introduced to capture also models like the Larson model within the framework.

When, for example, a long flexible polymer molecule is considered, the configuration distribution function for the equilibrium state is approximately Gaussian:

$$\psi_0(\vec{R}) = (\beta/\sqrt{\pi})^3 \exp(-\beta^2 R^2)$$

where \vec{R} is the end-to-end vector of the polymer chain, $R^2 = \vec{R} \cdot \vec{R}$ and $\beta^2 = 3/(2N_k b^2)$. N_k is the number of Kuhn steps, b the length of a Kuhn step. For a given end-to-end vector \vec{R} of a chain, the number of configurations Ω of that chain is proportional to $\psi_0(\vec{R})$.

Then the entropy is given by:

$$S = k \log(c\psi_0) = k(\log(c) + 3 \log(\beta/\sqrt{\pi}) - \beta^2 R^2)$$

For the free energy $W = -TS$, and $\delta W = \vec{f} \cdot \delta \vec{R}$, \vec{f} is the external force on the chain:

$$\vec{f} = 2kT\beta^2 \vec{R}$$

The average stress tensor based on this linear relation between the external force and the end-to-end vector (the element is a linear spring with a spring constant $2kT\beta^2$) is:

$$\sigma = 2\nu kT\beta^2 \langle \vec{R}\vec{R} \rangle$$

It is postulated that the average stress tensor of particles of type i , the contribution to the Cauchy stress tensor of these particles, can be expressed in this form (Non-linear spring behaviour will be discussed later):

$$\sigma_i = c \langle \vec{R}\vec{R} \rangle_i$$

For convenience the subscript i will be omitted. The constitutive equation for the length of the relevant structural element is postulated as:

$$\dot{\vec{R}} = \mathbf{L} \cdot \vec{R} - \mathbf{A} \cdot \vec{R}$$

The second order tensor \mathbf{A} is a yet to be specified function of averaged variables (for example stress, strain or strain rate).

The level of description, a vector representing a force carrying element on the micro level, is taken in an average sense. The vector $\dot{\vec{R}}$ does not include the actual rapid fluctuation of \vec{R} due to thermal motion; this motion is averaged out.

The term $-\mathbf{A} \cdot \dot{\vec{R}}$ represents the slippage of the element with respect to the continuum. Therefore \mathbf{A} is called the slip tensor. In case the relevant structural element deforms affine with the macroscopic deformation $\mathbf{A} = \mathbf{0}$. Notice that the above constitutive equation is postulated for any deformation and not for the special case of a sudden, steplike, deformation with no time for relaxation. This means that the equation for $\dot{\vec{R}}$ incorporates both convection and diffusion of \vec{R} .

Examples of the use of a similar expression for $\dot{\vec{R}}$, but restricted to the instantaneous response after a sudden deformation, i.e. describing only convective motion of \vec{R} , are (a) the one used for the differential approximation to the Doi–Edwards constitutive equation, (b) the Gordon–Schowalter nonaffine motion incorporated in the Johnson/Segalman model and in the Phan–Thien/Tanner model, and (c) the Larson nonaffine motion incorporated in the differential constitutive equation of Larson.:

$$(a) \quad \dot{\vec{R}} = \mathbf{L} \cdot \vec{R} - (\vec{n}\vec{n}:\mathbf{D})\vec{R}; \quad \vec{n} = \vec{R}/|\vec{R}|,$$

$$(b) \quad \dot{\vec{R}} = \mathbf{L} \cdot \vec{R} - \xi \mathbf{D} \cdot \vec{R},$$

$$(c) \quad \dot{\vec{R}} = \mathbf{L} \cdot \vec{R} - \xi(\vec{n}\vec{n}:\mathbf{D})\vec{R}; \quad \xi = \xi(\sigma); \quad \vec{n} = \vec{R}/|\vec{R}|.$$

A more general expression was used by Larson:

$$\dot{\vec{R}} = ({}^4\mathbf{Z}:\mathbf{L})\cdot\vec{R}$$

which can be rewritten to:

$$\dot{\vec{R}} = \mathbf{L}\cdot\vec{R} - [({}^4\mathbf{I} - {}^4\mathbf{Z}):\mathbf{L}]\cdot\vec{R}$$

With the abbreviation $\mathbf{A} = ({}^4\mathbf{I} - {}^4\mathbf{Z}):\mathbf{L}$ a similar expression for $\dot{\vec{R}}$ is obtained as proposed here.

The time derivative of the stress tensor is given by:

$$\dot{\sigma} = c(\langle\dot{\vec{R}}\vec{R}\rangle + \langle\vec{R}\dot{\vec{R}}\rangle)$$

Substitution of the expression for $\dot{\vec{R}}$ leaves us with:

$$\dot{\sigma} = c(\mathbf{L}\cdot\langle\vec{R}\vec{R}\rangle + \langle\vec{R}\vec{R}\rangle\cdot\mathbf{L}^c - \mathbf{A}\cdot\langle\vec{R}\vec{R}\rangle - \langle\vec{R}\vec{R}\rangle\cdot\mathbf{A}^c)$$

or, with the expression for σ :

$$\dot{\sigma} = \mathbf{L}\cdot\sigma + \sigma\cdot\mathbf{L} - \mathbf{A}\cdot\sigma - \sigma\cdot\mathbf{A}^c$$

which can be rewritten to the rather general constitutive equation for the stress tensor:

$$\dot{\hat{\sigma}} = \dot{\sigma} - \mathbf{L} \cdot \sigma - \sigma \cdot \mathbf{L}^c + \mathbf{A} \cdot \sigma + \sigma \cdot \mathbf{A}^c = 0$$

With the definition of the upper-convected time derivative:

$$\overset{\nabla}{\sigma} + \mathbf{A} \cdot \sigma + \sigma \cdot \mathbf{A}^c = 0$$

In terms of the extra stress tensor $\tau = \sigma - c\mathbf{I}$, using $\overset{\nabla}{\mathbf{I}} = -2\mathbf{D}$, the constitutive equation reads:

$$\overset{\nabla}{\tau} + \mathbf{A} \cdot \tau + \tau \cdot \mathbf{A}^c + c(\mathbf{A} + \mathbf{A}^c) = 2c\mathbf{D}$$

Specification of the slip tensor \mathbf{A} is possible by means of detailed microscopic modeling. Examples of such are bead-rod spring models.

The bead-spring model with hydrodynamic interaction leads to:

$$\dot{\vec{\mathbf{R}}}_i = \mathbf{L} \cdot \vec{\mathbf{R}}_i - \underline{\mathbf{A}}' \vec{\mathbf{f}} = \mathbf{L} \cdot \vec{\mathbf{R}}_i - \underline{\mathbf{A}}' \left[\kappa \vec{\mathbf{R}}_i + kT \frac{\partial}{\partial \vec{\mathbf{R}}_i} \ln(\psi(\vec{\mathbf{R}}_i, t)) \right]$$

where $\vec{\mathbf{R}}_i$ is the set of vectors connecting the beads in one chain and $\underline{\mathbf{A}}'$ is a modified Rouse matrix. Transformation to normal coordinates changes this to:

$$\dot{\vec{\mathbf{R}}}_i = \mathbf{L} \cdot \vec{\mathbf{R}}_i - \frac{a}{\zeta} \left[\kappa \vec{\mathbf{R}}_i + kT \frac{\partial}{\partial \vec{\mathbf{R}}_i} \ln(\psi(\vec{\mathbf{R}}_i, t)) \right]$$

The constitutive equation derived from this expression is the Upper Convected Maxwell model; a very restrictive model. If $\psi(\vec{R}_i, t)$ is specified, this expression can be transferred into a form that fits in the presented framework.

There are restrictions to the slip tensor \mathbf{A} . For example, \mathbf{A} should be chosen in a way that stress relaxation is described properly. When a flow is stopped, i.e. $\mathbf{L} = \mathbf{0}$, the constitutive equation reads:

$$\dot{\sigma} + \mathbf{A}(\mathbf{D}=\mathbf{0}) \cdot \sigma + \sigma \cdot \mathbf{A}^c(\mathbf{D}=\mathbf{0}) = \mathbf{0}$$

For the time $t \rightarrow \infty$, equilibrium will be attained and thus $\dot{\sigma} \rightarrow \mathbf{0}$, $\sigma \rightarrow c\mathbf{I}$ and therefore $\mathbf{A} \rightarrow \mathbf{0}$. Restricting \mathbf{A} to be a function of σ and \mathbf{D} , $\mathbf{A} = \mathbf{A}(\sigma, \mathbf{D})$, it follows:

$$\mathbf{A} = \mathbf{A}(\sigma, \mathbf{0}) = \mathbf{A}^* \rightarrow \mathbf{0} \text{ for } t \rightarrow \infty;$$

A quite general choice for \mathbf{A}^* which satisfies this requirement is of the form:

$$\mathbf{A}^* = \alpha_1 \sigma + \alpha_2 \sigma^{-1} + \alpha_3 \mathbf{I}; \quad -\alpha_3 \rightarrow c\alpha_1 + \alpha_2/c \text{ for } t \rightarrow \infty$$

where α_i are scalar functions of the invariants of σ . Notice that adding higher order terms of σ does not make sense as these terms can be expressed in σ , σ^{-1} and \mathbf{I} by the Cayley–Hamilton theorem. In case $\mathbf{A} = \mathbf{A}^*$ for all flows, the constitutive equation reads:

$$\dot{\sigma} + 2\alpha_1 \sigma \cdot \sigma + 2\alpha_2 \mathbf{I} + 2\alpha_3 \sigma = \mathbf{0}$$

The Leonov Model

If the stress tensor σ is related to the elastic strain tensor \mathbf{B}_e , the strain tensor which describes the change of shape of a material element during free recovery, according to classical rubber elasticity theory, i.e:

$$\sigma = G\mathbf{B}_e$$

and this relation is substituted in the expression for \mathbf{A}^* , then:

$$\mathbf{A}^* = \beta_1\mathbf{B}_e + \beta_2\mathbf{B}_e^{-1} + \beta_3\mathbf{I}; \quad -\beta_3 \rightarrow \beta_1 + \beta_2 \text{ for } t \rightarrow 0$$

For $\beta_1 = 1/4\lambda$, $\beta_2 = -G^2/4\lambda$ and $\beta_3 = (\mathbf{I}_1 - G^2\mathbf{I}_1)/12\lambda$ ($\mathbf{I}_1 = \text{tr}(\sigma)$, $\mathbf{I}_1^{-1} = \text{tr}(\sigma^{-1})$) the Leonov model is obtained:

$$\dot{\sigma} + \frac{1}{2G\lambda}[\sigma \cdot \sigma - G^2\mathbf{I} - \frac{1}{3}(\mathbf{I}_1 - G^2\mathbf{I}_1)\sigma] = 0$$

The tensor \mathbf{A}^* corresponds, in this case, to the irreversible rate of strain tensor \mathbf{D}_p in the Leonov model. The special choice for the constitutive equation for \mathbf{D}_p as proposed by Leonov is, in literature, often mentioned as seemingly arbitrary. However, it is shown that this choice provides a correct and quite general description of the phenomenon of stress relaxation.

In the following a number of examples is given of known models and extensions of some of these models are given.

Forms of the slip tensor \mathbf{A}

1) Classical rubber elasticity.

$$\mathbf{A} = \mathbf{0} \rightarrow \dot{\mathbf{R}} = \mathbf{L} \cdot \mathbf{R} \text{ (affine deformation)} \rightarrow \nabla \boldsymbol{\sigma} = \mathbf{0}$$

Notice, from the definition of the upper convected time derivative, that:

$$\nabla \mathbf{B} = \mathbf{0}$$

and therefore:

$$\boldsymbol{\sigma} = \mathbf{GB}$$

In terms of the extra stress tensor $\boldsymbol{\tau}$:

$$\nabla \boldsymbol{\sigma} = \nabla \boldsymbol{\tau} - 2\mathbf{GD} = \mathbf{0}$$

2) Upper convected Maxwell model (UCM).

$$\mathbf{A} = \alpha_1 \boldsymbol{\sigma} + \alpha_2 \boldsymbol{\sigma}^{-1} + \alpha_3 \mathbf{I}$$

$$\alpha_1 = 0; \quad \alpha_2 = -G/2\lambda \quad \alpha_3 = 1/2\lambda$$

$$\dot{\mathbf{R}} = \mathbf{L} \cdot \mathbf{R} - \left(\frac{1}{2\lambda} \mathbf{I} - \frac{G}{2\lambda} \boldsymbol{\sigma}^{-1} \right) \cdot \mathbf{R}$$

$$\nabla \boldsymbol{\sigma} + \frac{1}{\lambda} \boldsymbol{\sigma} - \frac{G}{\lambda} \mathbf{I} = \mathbf{0}$$

3) Lower convected Maxwell model (LCM).

$$\mathbf{A} = \mathbf{L} + \mathbf{L}^c + \alpha_1 \boldsymbol{\sigma} + \alpha_2 \boldsymbol{\sigma}^{-1} + \alpha_3 \mathbf{I} = 2\mathbf{D} + \alpha_1 \boldsymbol{\sigma} + \alpha_2 \boldsymbol{\sigma}^{-1} + \alpha_3 \mathbf{I}$$

$$\alpha_1 = 0; \quad \alpha_2 = -G/2\lambda \quad \alpha_3 = 1/2\lambda$$

$$\dot{\mathbf{R}} = \mathbf{L} \cdot \vec{\mathbf{R}} - \left(2\mathbf{D} + \frac{1}{2\lambda} \mathbf{I} - \frac{G}{2\lambda} \boldsymbol{\sigma}^{-1} \right) \cdot \vec{\mathbf{R}}$$

Notice: for a steplike deformation $\dot{\mathbf{R}} = \mathbf{L} \cdot \vec{\mathbf{R}} - 2\mathbf{D} \cdot \vec{\mathbf{R}} = (-\mathbf{D} + \boldsymbol{\Omega}) \cdot \vec{\mathbf{R}}$.

The structural element shortens during a macroscopic extension of the continuum. This seems to be not very realistic.

$$\Delta \boldsymbol{\sigma} + \frac{1}{\lambda} \boldsymbol{\sigma} - \frac{G}{\lambda} \mathbf{I} = \mathbf{0}$$

4) Corotational Maxwell model (CM).

$$\mathbf{A} = \mathbf{D} + \alpha_1 \boldsymbol{\sigma} + \alpha_2 \boldsymbol{\sigma}^{-1} + \alpha_3 \mathbf{I}$$

$$\alpha_1 = 0; \quad \alpha_2 = -G/2\lambda \quad \alpha_3 = 1/2\lambda$$

$$\dot{\mathbf{R}} = \mathbf{L} \cdot \vec{\mathbf{R}} - \left(\mathbf{D} + \frac{1}{2\lambda} \mathbf{I} - \frac{G}{2\lambda} \boldsymbol{\sigma}^{-1} \right) \cdot \vec{\mathbf{R}}$$

$$\overset{\circ}{\boldsymbol{\sigma}} + \frac{1}{\lambda} \boldsymbol{\sigma} - \frac{G}{\lambda} \mathbf{I} = \mathbf{0}$$

5) Oldroyd B.

$$\text{UCM \& } \sigma_s = 2\eta_s \mathbf{D}$$

6) Oldroyd A.

$$\text{LCM \& } \sigma_s = 2\eta_s \mathbf{D}$$

7) Johnson Segelman.

$$\mathbf{A} = \xi \mathbf{D} + \alpha_1 \boldsymbol{\sigma} + \alpha_2 \boldsymbol{\sigma}^{-1} + \alpha_3 \mathbf{I}$$

$$\alpha_1 = 0; \quad \alpha_2 = -G/2\lambda \quad \alpha_3 = 1/2\lambda$$

$$\dot{\mathbf{R}} = \mathbf{L} \cdot \mathbf{R} - \left(\xi \mathbf{D} + \frac{1}{2\lambda} \mathbf{I} - \frac{G}{2\lambda} \boldsymbol{\sigma}^{-1} \right) \cdot \mathbf{R}$$

$$\nabla \boldsymbol{\sigma} + \xi (\boldsymbol{\sigma} \cdot \mathbf{D} + \mathbf{D} \cdot \boldsymbol{\sigma}) + \frac{1}{\lambda} \boldsymbol{\sigma} - \frac{G}{\lambda} \mathbf{I} = 0$$

8) Doi/Edwards, the differential approximation.

$$\mathbf{A} = \frac{1}{3G}(\boldsymbol{\sigma}:\mathbf{D})\mathbf{I} + \alpha_1\boldsymbol{\sigma} + \alpha_2\boldsymbol{\sigma}^{-1} + \alpha_3\mathbf{I}$$

$$\alpha_1=0; \quad \alpha_2 = -G/2\lambda \quad \alpha_3 = 1/2\lambda$$

$$\dot{\vec{\mathbf{R}}} = \mathbf{L}\cdot\vec{\mathbf{R}} - \left(\frac{1}{3G}(\boldsymbol{\sigma}:\mathbf{D})\mathbf{I} + \frac{1}{2\lambda}\mathbf{I} - \frac{G}{2\lambda}\boldsymbol{\sigma}^{-1}\right)\cdot\vec{\mathbf{R}}$$

$$\dot{\boldsymbol{\sigma}} + \frac{2}{3G}(\boldsymbol{\sigma}:\mathbf{D})\boldsymbol{\sigma} + \frac{1}{\lambda}\boldsymbol{\sigma} - \frac{G}{\lambda}\mathbf{I} = 0$$

The original approximation starts with:

$$\dot{\vec{\mathbf{R}}} = \mathbf{L}\cdot\vec{\mathbf{R}} - \vec{\mathbf{n}}\vec{\mathbf{n}}:\mathbf{D}\vec{\mathbf{R}}; \quad \vec{\mathbf{n}} = \vec{\mathbf{R}}/|\vec{\mathbf{R}}|$$

for a steplike deformation. This equation expresses that the end-to-end vector only rotates and does not extend. For a steplike deformation, the constitutive equation for $\dot{\vec{\mathbf{R}}}$ as used here, becomes:

$$\dot{\vec{\mathbf{R}}} = \mathbf{L}\cdot\vec{\mathbf{R}} - \frac{1}{3G}(\boldsymbol{\sigma}:\mathbf{D})\vec{\mathbf{R}}$$

Substitution of the equation for the stress tensor for the Doi/Edwards model:

$$\sigma = 3G \frac{1}{|\vec{R}|^2} \langle \vec{R}\vec{R} \rangle = 3G \langle \vec{nn} \rangle$$

gives

$$\dot{\vec{R}} = \mathbf{L} \cdot \vec{R} - \langle \vec{nn} \rangle : \mathbf{D} \vec{R}$$

Thus, the original equation for $\dot{\vec{R}}$ is replaced by one with a pre-averaged tensor $\langle \vec{nn} \rangle$ which still gives the same final result.

9) Doi/Edwards, the extended differential approximation. If it is stated that the relaxation time λ decreases with increasing strain rate and/or stress, and this relaxation time is defined by:

$$\lambda = \lambda_0 / \left[\frac{2\lambda_0}{3G} \sigma : \mathbf{D} + 1 \right]$$

Substitution in a UCM model leads to:

$$\mathbf{A} = \frac{1}{3G} (\sigma : \mathbf{D}) \mathbf{I} - \frac{1}{3} (\sigma : \mathbf{D}) \sigma^{-1} + \alpha_1 \sigma + \alpha_2 \sigma^{-1} + \alpha_3 \mathbf{I}$$

$$\alpha_1 = 0; \quad \alpha_2 = -G/2\lambda \quad \alpha_3 = 1/2\lambda$$

$$\dot{\vec{R}} = \mathbf{L} \cdot \vec{R} - \left(\frac{1}{3G} (\sigma : \mathbf{D}) \mathbf{I} - \frac{1}{3} (\sigma : \mathbf{D}) \sigma^{-1} + \frac{1}{2\lambda_0} \mathbf{I} - \frac{G}{2\lambda_0} \sigma^{-1} \right) \cdot \vec{R}$$

$$\mathbf{V} \sigma + \left[\frac{2}{3G} (\sigma : \mathbf{D}) + 1 \right] \sigma - \left[\frac{G}{\lambda_0} \frac{1}{3} \sigma : \mathbf{D} + \frac{1}{\lambda_0} \right] \mathbf{I} = \mathbf{0}$$

This is called the Doi/Edwards extended differential approximation. Notice that for a step strain there will be some stretching of the structural element which is not the case for the original Doi/Edwards differential approximation where only rotation of the elements takes place. The extended model seems therefore to be more realistic as a steplike deformation leads to deformation of the structural element. Also, the overshoot in the first normal stress difference as found in start-up of simple shear experiments, which is not predicted by the original model, is predicted when stretching is incorporated in the model (Larson 1988, Geffroy and Leal (1992)).

The definition of the relaxation time λ is a mix of the WM model and the MUCM model.

10) Larson, partially extending; the original and the correct version.

$$\mathbf{A} = \left[\frac{\xi}{\text{tr}(\boldsymbol{\sigma})} + \delta \frac{6G\xi(1-\xi)}{\text{tr}^2(\boldsymbol{\sigma})} \right] (\boldsymbol{\sigma}:\mathbf{D})\mathbf{I} + \alpha_1\boldsymbol{\sigma} + \alpha_2\boldsymbol{\sigma}^{-1} + \alpha_3\mathbf{I}$$

$$\alpha_1 = 0; \quad \alpha_2 = -G/2\lambda \quad \alpha_3 = 1/2\lambda$$

original version: $\delta = 0$; correct version: $\delta = 1$

$$\dot{\mathbf{R}} = \mathbf{L} \cdot \mathbf{R} - \left[\frac{\xi}{\text{tr}(\boldsymbol{\sigma})} + \delta \frac{6G\xi(1-\xi)}{\text{tr}^2(\boldsymbol{\sigma})} \right] (\boldsymbol{\sigma}:\mathbf{D})\mathbf{I} + \frac{1}{2\lambda}\mathbf{I} - \frac{G}{2\lambda}\boldsymbol{\sigma}^{-1} \cdot \mathbf{R}$$

$$\mathbf{V} \cdot \boldsymbol{\sigma} + 2 \left[\frac{\xi}{\text{tr}(\boldsymbol{\sigma})} + \delta \frac{6G\xi(1-\xi)}{\text{tr}^2(\boldsymbol{\sigma})} \right] (\boldsymbol{\sigma}:\mathbf{D})\boldsymbol{\sigma} + \frac{1}{\lambda}\boldsymbol{\sigma} - \frac{G}{\lambda}\mathbf{I} = 0$$

11) Larson, simplified partially extending.

$$\mathbf{A} = \left[\frac{\xi}{3G} + \delta \frac{2\xi(1-\xi)}{3G} \right] (\boldsymbol{\sigma} : \mathbf{D}) \mathbf{I} + \alpha_1 \boldsymbol{\sigma} + \alpha_2 \boldsymbol{\sigma}^{-1} + \alpha_3 \mathbf{I}$$

$$\alpha_1 = 0; \quad \alpha_2 = -G/2\lambda \quad \alpha_3 = 1/2\lambda$$

original version: $\delta = 0$; correct version: $\delta = 1$

$$\dot{\mathbf{R}} = \mathbf{L} \cdot \dot{\mathbf{R}} - \left(\left[\frac{\xi}{3G} + \delta \frac{2\xi(1-\xi)}{3G} \right] (\boldsymbol{\sigma} : \mathbf{D}) \mathbf{I} + \frac{1}{2\lambda} \mathbf{I} - \frac{G}{2\lambda} \boldsymbol{\sigma}^{-1} \right) \cdot \dot{\mathbf{R}}$$

$$\mathbb{V} \boldsymbol{\sigma} + \left[\frac{2\xi}{3G} + \delta \frac{4\xi(1-\xi)}{3G} \right] (\boldsymbol{\sigma} : \mathbf{D}) \boldsymbol{\sigma} + \frac{1}{\lambda} \boldsymbol{\sigma} - \frac{G}{\lambda} \mathbf{I} = 0$$

12) Larson, irreversible.

$$\mathbf{A} = \left[\frac{\xi}{t \mathbf{I}(\boldsymbol{\sigma})} + \delta \frac{6G\xi(1-\xi)}{t \mathbf{I}^2(\boldsymbol{\sigma})} \right] [(\boldsymbol{\sigma} : \mathbf{D})]_+ \mathbf{I} + \alpha_1 \boldsymbol{\sigma} + \alpha_2 \boldsymbol{\sigma}^{-1} + \alpha_3 \mathbf{I};$$

$$[(\boldsymbol{\sigma} : \mathbf{D})]_+ = \boldsymbol{\sigma} : \mathbf{D} \text{ for } \boldsymbol{\sigma} : \mathbf{D} \geq 0; \quad [(\boldsymbol{\sigma} : \mathbf{D})]_+ = 0 \text{ for } \boldsymbol{\sigma} : \mathbf{D} \leq 0$$

$$\alpha_1 = 0; \quad \alpha_2 = -G/2\lambda \quad \alpha_3 = 1/2\lambda$$

original version: $\delta = 0$; correct version: $\delta = 1$

$$\dot{\mathbf{R}} = \mathbf{L} \cdot \dot{\mathbf{R}} - \left(\left[\frac{\xi}{t \mathbf{I}(\boldsymbol{\sigma})} + \delta \frac{6G\xi(1-\xi)}{t \mathbf{I}^2(\boldsymbol{\sigma})} \right] [(\boldsymbol{\sigma} : \mathbf{D})]_+ \mathbf{I} + \frac{1}{2\lambda} \mathbf{I} - \frac{G}{2\lambda} \boldsymbol{\sigma}^{-1} \right) \cdot \dot{\mathbf{R}}$$

$$\mathbb{V} \boldsymbol{\sigma} + 2 \left[\frac{\xi}{t \mathbf{I}(\boldsymbol{\sigma})} + \delta \frac{6G\xi(1-\xi)}{t \mathbf{I}^2(\boldsymbol{\sigma})} \right] [(\boldsymbol{\sigma} : \mathbf{D})]_+ \boldsymbol{\sigma} + \frac{1}{\lambda} \boldsymbol{\sigma} - \frac{G}{\lambda} \mathbf{I} = 0$$

13) Giesekus.

$$\mathbf{A} = \alpha_1 \boldsymbol{\sigma} + \alpha_2 \boldsymbol{\sigma}^{-1} + \alpha_3 \mathbf{I}$$

$$\alpha_1 = \frac{\alpha}{2\lambda G}; \quad \alpha_2 = -\frac{G}{2\lambda}(1-\alpha); \quad \alpha_3 = \frac{1}{2\lambda}(1-2\alpha)$$

$$\dot{\mathbf{R}} = \mathbf{L} \cdot \dot{\mathbf{R}} - \left(\frac{1}{2\lambda}(1-2\alpha)\mathbf{I} - \frac{G}{2\lambda}(1-\alpha)\boldsymbol{\sigma}^{-1} \right) \cdot \dot{\mathbf{R}}$$

$$\nabla \cdot \boldsymbol{\sigma} + \frac{\alpha}{\lambda G} \boldsymbol{\sigma} \cdot \boldsymbol{\sigma} + \frac{1}{\lambda}(1-2\alpha)\boldsymbol{\sigma} - \frac{G}{\lambda}(1-\alpha)\mathbf{I} = \mathbf{0}$$

15) Leonov.

$$\mathbf{A} = \alpha_1 \boldsymbol{\sigma} + \alpha_2 \boldsymbol{\sigma}^{-1} + \alpha_3 \mathbf{I}$$

$$\alpha_1 = \frac{1}{4\lambda G}; \quad \alpha_2 = -\frac{G}{4\lambda}; \quad \alpha_3 = (\mathbf{I}_1 - G^2 \mathbf{I}_1) / 12\lambda \quad (\mathbf{I}_1 = \text{tr}(\boldsymbol{\sigma}), \mathbf{I}_1 = \text{tr}(\boldsymbol{\sigma}^{-1}))$$

$$\dot{\mathbf{R}} = \mathbf{L} \cdot \dot{\mathbf{R}} - \left(\frac{1}{4\lambda G} \boldsymbol{\sigma} - \frac{G}{4\lambda} \boldsymbol{\sigma}^{-1} + \frac{(\mathbf{I}_1 - \mathbf{I}_1)}{12\lambda} \mathbf{I} \right) \cdot \dot{\mathbf{R}}$$

$$\nabla \cdot \boldsymbol{\sigma} + \frac{1}{2G\lambda} [\boldsymbol{\sigma} \cdot \boldsymbol{\sigma} - G^2 \mathbf{I} - \frac{1}{3}(\mathbf{I}_1 - G^2 \mathbf{I}_1) \boldsymbol{\sigma}] = \mathbf{0}$$

16) Phan-Thien/Tanner a & b

$$\mathbf{A} = \xi \mathbf{D} + \alpha_1 \boldsymbol{\sigma} + \alpha_2 \boldsymbol{\sigma}^{-1} + \alpha_3 \mathbf{I}$$

$$\alpha_1 = 0; \quad \alpha_2 = -G/2\lambda \quad \alpha_3 = 1/2\lambda \quad \lambda = \lambda(\text{tr}(\boldsymbol{\sigma}))$$

$$\dot{\mathbf{R}} = \mathbf{L} \cdot \dot{\mathbf{R}} - \left(\xi \mathbf{D} + \frac{1}{2\lambda} \mathbf{I} - \frac{G}{2\lambda} \boldsymbol{\sigma}^{-1} \right) \cdot \dot{\mathbf{R}}$$

$$\nabla \boldsymbol{\sigma} + \xi (\mathbf{D} \cdot \boldsymbol{\sigma} + \boldsymbol{\sigma} \mathbf{D}) + \frac{1}{\lambda} \boldsymbol{\sigma} - \frac{G}{\lambda} \mathbf{I} = \mathbf{0}$$

$$\text{PTT-a: } \lambda = \lambda_0 \exp\left(-\frac{\epsilon}{G} \text{tr}(\boldsymbol{\sigma} - \mathbf{G}\mathbf{I})\right)$$

$$\text{PTT-b: } \lambda = \lambda_0 \left(1 + \frac{\epsilon}{G} \text{tr}(\boldsymbol{\sigma} - \mathbf{G}\mathbf{I})\right)^{-1}$$

17) White Metzner.

$$\mathbf{A} = \alpha_1 \boldsymbol{\sigma} + \alpha_2 \boldsymbol{\sigma}^{-1} + \alpha_3 \mathbf{I}$$

$$\alpha_1 = 0; \quad \alpha_2 = -G/2\lambda; \quad \alpha_3 = 1/2\lambda; \quad \lambda = \lambda(\Pi_{\mathbf{D}}) = \frac{\lambda_0}{1 + \frac{\lambda_0}{\alpha \lambda_0 \nu} \Pi_{\mathbf{D}}}$$

$$\dot{\mathbf{R}} = \mathbf{L} \cdot \dot{\mathbf{R}} - \left(\frac{1}{2\lambda} \mathbf{I} - \frac{G}{2\lambda} \boldsymbol{\sigma}^{-1} \right) \cdot \dot{\mathbf{R}}$$

$$\nabla \boldsymbol{\sigma} + \frac{1}{\lambda} \boldsymbol{\sigma} - \frac{G}{\lambda} \mathbf{I} = \mathbf{0}$$

18) MUCM, Modified UCM (equivalent to PTT-b).

$$\alpha_1 = 0; \quad \alpha_2 = -G/2\lambda; \quad \alpha_3 = 1/2\lambda; \quad \lambda = \lambda(I_{\boldsymbol{\sigma}}) = \frac{\lambda_0}{1 + \frac{\lambda_0}{F} \text{tr}(\boldsymbol{\sigma} - \mathbf{G}\mathbf{I})}$$

$$\dot{\mathbf{R}} = \mathbf{L} \cdot \dot{\mathbf{R}} - \left(\frac{1}{2\lambda} \mathbf{I} - \frac{G}{2\lambda} \boldsymbol{\sigma}^{-1} \right) \cdot \dot{\mathbf{R}}$$

$$\nabla \boldsymbol{\sigma} + \frac{1}{\lambda} \boldsymbol{\sigma} - \frac{G}{\lambda} \mathbf{I} = \mathbf{0}$$

19) FENE-P, Peterlin approximation for FENE dumbbells.

$$\mathbf{A} = \alpha_1 \boldsymbol{\sigma} + \alpha_2 \boldsymbol{\sigma}^{-1} + \alpha_3 \mathbf{I}$$

$$\alpha_1 = 0; \quad \alpha_2 = -\frac{Z}{2\lambda} G; \quad \alpha_3 = \frac{1}{2} \left(\frac{Z}{\lambda} - \frac{\dot{Z}}{Z} \right); \quad G = G_0(1-\epsilon b); \quad G_0 = \nu kT$$

$$\epsilon = \frac{2}{b(b+2)}; \quad b = \frac{HQ_0^2}{kT};$$

$$Z = 1 + \frac{3}{b}((1-\epsilon b) + \frac{1}{3G_0} \text{tr}(\boldsymbol{\sigma} - G_0(1-\epsilon b)\mathbf{I})) = 1 + \frac{1}{bG_0} \text{tr}(\boldsymbol{\sigma})$$

$$\dot{Z} = \frac{1}{bG_0} \text{tr}(\dot{\boldsymbol{\sigma}})$$

$$\dot{\mathbf{R}} = \mathbf{L} \cdot \dot{\mathbf{R}} - \left(\frac{1}{2} \left(\frac{Z}{\lambda} - \frac{\dot{Z}}{Z} \right) \mathbf{I} - \frac{Z}{2\lambda} G \boldsymbol{\sigma}^{-1} \right) \cdot \dot{\mathbf{R}}$$

$$\nabla \boldsymbol{\sigma} + \left(\frac{Z}{\lambda} - \frac{\dot{Z}}{Z} \right) \boldsymbol{\sigma} - \frac{Z}{\lambda} G \mathbf{I} = 0$$

This is the approximate constitutive equation for FENE Dumbbells. This equation can be rewritten so it is more easy to compare with results obtained with the framework presented. Using the expression for $\dot{\boldsymbol{\sigma}}$ for structural elements with a non-linear spring behaviour one gets:

$$\text{tr}(\dot{\boldsymbol{\sigma}}) = \mathbf{I} : \dot{\boldsymbol{\sigma}} = \mathbf{I} : [(\mathbf{L} - \mathbf{A}_k) \cdot \boldsymbol{\sigma} + \boldsymbol{\sigma} \cdot (\mathbf{L}^c - \mathbf{A}_k)]; \quad \mathbf{A}_k = \mathbf{A} - K(\mathbf{D} : \boldsymbol{\sigma} - \mathbf{A} : \boldsymbol{\sigma})\mathbf{I}$$

$$\text{tr}(\dot{\boldsymbol{\sigma}}) = 2(1 + K\mathbf{I} : \boldsymbol{\sigma})(\mathbf{D} : \boldsymbol{\sigma} - \mathbf{A} : \boldsymbol{\sigma}); \quad K = \frac{1}{bG_0}$$

This leads to:

$$\frac{\dot{Z}}{Z} = \frac{2}{bG_0} (\mathbf{D} - \mathbf{A}) : \boldsymbol{\sigma}$$

Now the slip tensor has to be specified. Notice that one has the freedom to combine the FENE-P model with different slip models. Here, the slip tensor is chosen according to the model of Larson which describes partial extending of the structural elements:

$$\mathbf{A} = \left[\frac{\xi}{\text{tr}(\boldsymbol{\sigma})} + \delta \frac{6G\xi(1-\xi)}{\text{tr}^2(\boldsymbol{\sigma})} \right] (\boldsymbol{\sigma} \cdot \mathbf{D}) \mathbf{I} - \frac{G}{2\lambda} \boldsymbol{\sigma}^{-1} + \frac{1}{2\lambda} \mathbf{I}$$

With $\delta = 0$ it follows that:

$$\frac{\dot{\mathbf{Z}}}{\lambda} - \frac{\dot{\mathbf{Z}}}{\mathbf{Z}} = \frac{1}{\lambda} (1 + 2K \text{tr}(\boldsymbol{\sigma}) - 3KG) - 2K(1-\xi) \boldsymbol{\sigma} \cdot \mathbf{D}$$

which gives the constitutive equation as:

$$\dot{\boldsymbol{\sigma}} + \left[\frac{1}{\lambda} (1 + 2K \text{tr}(\boldsymbol{\sigma}) - 3KG) - 2K(1-\xi) \boldsymbol{\sigma} \cdot \mathbf{D} \right] \boldsymbol{\sigma} - \frac{G}{\lambda} (1 + K \text{tr}(\boldsymbol{\sigma})) \mathbf{I} = \mathbf{0}$$

For $K = 0$ the UCM model is obtained. It is not possible, starting with this constitutive equation, to obtain Larsons original model which is based on linear springs. When a similar model is constructed within the proposed framework it is indeed possible to obtain the more simple underlying models by giving parameters the right values. The constitutive equation is then, using the same slip tensor \mathbf{A} , given by:

$$\dot{\boldsymbol{\sigma}} + \left[\frac{1}{\lambda} (1 + K \text{tr}(\boldsymbol{\sigma}) - 3KG) - 2K(1-\xi(1 + \frac{1}{K\text{tr}(\boldsymbol{\sigma})})) \boldsymbol{\sigma} \cdot \mathbf{D} \right] \boldsymbol{\sigma} - \frac{G}{\lambda} \mathbf{I} = \mathbf{0}$$

The previous version of the FENE-P model differs in two ways compared to latter. First the two terms:

$$\frac{1}{\lambda} K \text{tr}(\boldsymbol{\sigma}) \boldsymbol{\sigma} - \frac{G}{\lambda} K \text{tr}(\boldsymbol{\sigma}) \mathbf{I}$$

and the factor scaling the slip factor ξ in the latter:

$$1 + \frac{1}{K \text{tr}(\sigma)}$$

which makes that the Larson model is incorporated ($K=0$).

20) A more general nonseparable differential equation.

$$\nabla_{\tau} + a\tau^2 + b\tau + c\mathbf{I} = 2\eta\mathbf{D}$$

where a, b, c are functions of the invariants of τ .

PTT $\rightarrow \xi = 0$, $a = 0$, $b = (1 + \alpha \text{tr}(\tau))^{-1}$, $c = 0$.

STRUCTURAL ELEMENTS WITH A NON-LINEAR SPRING BEHAVIOUR

It was postulated that the average stress tensor of particles of type i , the contribution to the Cauchy stress tensor of these particles, can be expressed in the form:

$$\sigma_i = c \langle \vec{R}\vec{R} \rangle_i$$

in which c is a constant. This relation is based on a linear relation between the external force on the structural element and the end-to-end vector of the element. For convenience the subscript i will be omitted.

A more general expression, allowing for a non-linear relation between the external force \vec{f} and the end-to-end vector \vec{R} , is:

$$\sigma = \nu \langle \vec{f}(|\vec{R}|) \vec{R} \rangle = \nu \langle c(|\vec{R}|) \vec{R}\vec{R} \rangle$$

The time derivative of the stress tensor is given by:

$$\dot{\sigma} = \nu (\langle \dot{c} \vec{R}\vec{R} \rangle + \langle c \dot{\vec{R}}\vec{R} \rangle + \langle c \vec{R}\dot{\vec{R}} \rangle)$$

Substitution of the expression for $\dot{\vec{R}} = \mathbf{L} \cdot \vec{R} - \mathbf{A} \cdot \vec{R}$ leads to:

$$\dot{\sigma} = \nu (\mathbf{L} \cdot \langle c \vec{R}\vec{R} \rangle + \langle c \vec{R}\vec{R} \rangle \cdot \mathbf{L}^c - \mathbf{A} \cdot \langle c \vec{R}\vec{R} \rangle - \langle c \vec{R}\vec{R} \rangle \cdot \mathbf{A}^c + \langle \dot{c} \vec{R}\vec{R} \rangle)$$

or, with the expression for σ and the definition of the upper-convected time derivative:

$$\overset{\nabla}{\sigma} + \mathbf{A} \cdot \sigma + \sigma \cdot \mathbf{A}^c - \nu \langle \frac{\dot{c}}{c} c \vec{R}\vec{R} \rangle = \mathbf{0}$$

With the approximation:

$$\langle \frac{\dot{c}}{c} c \vec{R} \vec{R} \rangle \approx \langle \frac{\dot{c}}{c} \rangle \langle c \vec{R} \vec{R} \rangle$$

the constitutive equation reads:

$$\nabla \cdot \sigma + \mathbf{A} \cdot \sigma + \sigma \cdot \mathbf{A}^c - \langle \frac{\dot{c}}{c} \rangle \sigma = 0$$

The term $\langle \frac{\dot{c}}{c} \rangle$ can be worked out as:

$$\langle \frac{\dot{c}}{c} \rangle = \left\langle \frac{1}{c} \frac{\partial c}{\partial |\dot{\mathbf{R}}|} |\dot{\mathbf{R}}| \right\rangle = \left\langle \frac{1}{c^2} \frac{\partial c}{\partial |\dot{\mathbf{R}}|} \frac{1}{2|\dot{\mathbf{R}}|} \mathbf{I} : (c \dot{\mathbf{R}} \dot{\mathbf{R}} + c \dot{\mathbf{R}} \dot{\mathbf{R}}) \right\rangle$$

Or, with the expression for $\dot{\mathbf{R}}$:

$$\langle \frac{\dot{c}}{c} \rangle = \frac{1}{\nu} \left\langle \frac{1}{c^2} \frac{\partial c}{\partial |\dot{\mathbf{R}}|} \frac{1}{2|\dot{\mathbf{R}}|} \right\rangle \mathbf{I} : (\mathbf{L} \cdot \sigma + \sigma \cdot \mathbf{L}^c - \mathbf{A} \cdot \sigma - \sigma \cdot \mathbf{A}^c)$$

Using the definition for the non-linearity function K:

$$\mathbf{K} = \frac{1}{\nu} \left\langle \frac{1}{c^2} \frac{\partial c}{\partial |\dot{\mathbf{R}}|} \frac{1}{2|\dot{\mathbf{R}}|} \right\rangle$$

the constitutive equation for the stress tensor can be rewritten as:

$$\nabla \cdot \sigma + \mathbf{A} \cdot \sigma + \sigma \cdot \mathbf{A}^c - \mathbf{K} \mathbf{I} : (\mathbf{L} \cdot \sigma + \sigma \cdot \mathbf{L}^c - \mathbf{A} \cdot \sigma - \sigma \cdot \mathbf{A}^c) \sigma = 0$$

or, in a similar form as in the case for linear springs:

$$\dot{\sigma} + [\mathbf{A} - \mathbf{K}(\mathbf{D}:\sigma - \mathbf{A}:\sigma)\mathbf{I}] \cdot \sigma + \sigma \cdot [\mathbf{A}^c - \mathbf{K}(\mathbf{D}:\sigma - \mathbf{A}:\sigma)\mathbf{I}] = 0$$

It is assumed that the averaged function \mathbf{K} can be expressed in terms of averaged variables (for example stress, strain or strain rate).

With:

$$\mathbf{A}_k = \mathbf{A} - \mathbf{K}(\mathbf{D}:\sigma - \mathbf{A}:\sigma)\mathbf{I}$$

the constitutive equation reads:

$$\dot{\sigma} + \mathbf{A}_k \cdot \sigma + \sigma \cdot \mathbf{A}_k^c = 0$$

In terms of the extra stress tensor $\tau = \sigma - c\mathbf{I}$, using $\dot{\mathbf{I}} = -2\mathbf{D}$:

$$\dot{\tau} + \mathbf{A}_k \cdot \tau + \tau \cdot \mathbf{A}_k^c + 2c(\mathbf{A}_k + \mathbf{A}_k^c) = 2c\mathbf{D}$$

Notice that the final form of the constitutive equation for structural elements that behave as non-linear springs is identically to that for linear springs. This means that non-linear spring behaviour and nonaffine motion of the structural elements are equivalent; the tensor \mathbf{A}_k can be interpreted as the slip tensor in the constitutive equation for $\dot{\mathbf{R}}$.

It is illustrative to demonstrate the case that $\mathbf{K} = \text{constant}$ for each structural element.

Then, for the non-linearity function K it holds:

$$K^* = \nu K = \frac{1}{c^2} \frac{\partial c}{\partial |\vec{R}|} \frac{1}{2|\vec{R}|}$$

Solving this leads to an expression for the force in a structural element:

$$\vec{f} = \frac{1}{b - K^* |\vec{R}|^2} \vec{R}$$

where b is an integration constant. If it is assumed that $K > 0$, this expression has the same form as the approximation, as proposed by Warner, for the inverse Langevin function:

$$\vec{f} = \frac{2\beta^2 kT}{1 - (|\vec{R}|/|\vec{R}_{\max}|)^2} \vec{R}$$

The inverse Langevin function is a mathematically complex function which describes the force-extension relation for a freely jointed chain with many bonds, representing long molecules. Molecules can only be extended to their maximum length. The force-extension relation is therefore non-linear; the force becomes very large as the maximum length is approached. Comparing both expressions it follows for the integration constant b and the non-linearity function K:

$$b = \frac{1}{2\beta^2 kT}; \quad \frac{K^*}{b} = \frac{3GKT}{\langle \vec{R} \rangle_0^2}$$

Thus, by choosing $K = \text{constant}$ the model describes a finite extensible structural element. Notice that without specifying \mathbf{A} we found parts of \mathbf{A}_k which are similar to terms in the Larson model.

On the other hand, looking at the expression for A_k , the slip tensor A has to be specified. When A and K are specified as:

$$A = \frac{1}{2\lambda} \mathbf{I} - \frac{G}{2\lambda} \sigma^{-1}; \quad K = -\frac{\xi}{3G}$$

and, corresponding to Larson, $\text{tr}(\sigma)$ is replaced by a constant $3G$, it follows that A_k equals:

$$A_k = \frac{\xi}{3G}(\sigma:D)\mathbf{I} + \frac{1}{2\lambda} \mathbf{I} - \frac{G}{2\lambda} \sigma^{-1}$$

which is equal to the slip tensor A specified for the Larsons simplified partially extending model. In other words, the slip parameter ξ in the model of Larson, which is based on linear spring behaviour of the structural elements, can also be interpreted as a non-linearity parameter which takes into account non-linear spring behaviour.

For the case the non-linearity function K is chosen as:

$$K = -\left(\frac{\xi}{\text{tr}(\sigma)} + \frac{3G\xi(1-\xi)}{2 \text{tr}^2(\sigma)}\right)$$

and the slip tensor A as:

$$A = g(\sigma) \mathbf{I} - \frac{G}{2\lambda} \sigma^{-1}; \quad g(\sigma) = -\frac{1}{2\lambda} \frac{1-3GK}{1-\text{tr}(\sigma)K}$$

the correct version of Larsons partially extending model is obtained. Again, using the approximation $\text{tr}(\sigma) = 3G$, the improved version of Larsons simplified partially extending model is obtained

A MIXED STRESS TENSOR

From the constitutive equation for the rate of the end-to-end vector \vec{R} as proposed by Larson:

$$\dot{\vec{R}} = \mathbf{L} \cdot \vec{R} - \xi(\vec{n}\vec{n}:\mathbf{D}) \vec{R}; \quad \vec{n} = \vec{R}/|\vec{R}|$$

the corresponding stress tensor is found to be:

$$\sigma = \sigma_s + \sigma_c = A\langle\vec{R}\vec{R}\rangle + B\langle\vec{n}\vec{n}\rangle; \quad A = 2G\beta^2(1-\xi); \quad B = 3G\xi; \quad G = \nu kT$$

The derivation of the constitutive equation, based on the formulism as applied in this study starts with the time derivative of the stress tensor:

$$\dot{\sigma} = \dot{\sigma}_s + \dot{\sigma}_c = A(\langle\dot{\vec{R}}\vec{R}\rangle + \langle\vec{R}\dot{\vec{R}}\rangle) + B(\langle\dot{\vec{n}}\vec{n}\rangle + B\langle\vec{n}\dot{\vec{n}}\rangle)$$

The time derivative $\dot{\vec{n}}$ is, with $\dot{\vec{R}} = (\mathbf{L} - \mathbf{A}) \cdot \vec{R}$:

$$\dot{\vec{n}} = \frac{1}{|\vec{R}|}(\mathbf{I} - \vec{n}\vec{n}) \cdot \dot{\vec{R}} = \frac{1}{|\vec{R}|}(\mathbf{I} - \vec{n}\vec{n}) \cdot (\mathbf{L} - \mathbf{A}) \cdot \vec{R} = (\mathbf{I} - \vec{n}\vec{n}) \cdot (\mathbf{L} - \mathbf{A}) \cdot \vec{n}$$

Using this in the expression for the time derivative $\dot{\sigma}$ gives:

$$\dot{\sigma} = \dot{\sigma}_s + \dot{\sigma}_c = (\mathbf{L} - \mathbf{A}) \cdot \mathbf{A} \langle \vec{\mathbf{R}} \vec{\mathbf{R}} \rangle + \mathbf{A} \langle \vec{\mathbf{R}} \vec{\mathbf{R}} \rangle \cdot (\mathbf{L} - \mathbf{A})^c + \\ \langle (\mathbf{L} - \vec{\mathbf{n}} \vec{\mathbf{n}} : (\mathbf{L} - \mathbf{A}) \mathbf{I} + \mathbf{A}) \cdot \mathbf{B} \vec{\mathbf{n}} \vec{\mathbf{n}} \rangle + \langle \mathbf{B} \vec{\mathbf{n}} \vec{\mathbf{n}} \cdot (\mathbf{L} - \vec{\mathbf{n}} \vec{\mathbf{n}} : (\mathbf{L} - \mathbf{A}) \mathbf{I} + \mathbf{A})^c \rangle$$

With the approximation:

$$\langle (\mathbf{L} - \vec{\mathbf{n}} \vec{\mathbf{n}} : (\mathbf{L} - \mathbf{A}) \mathbf{I} + \mathbf{A}) \cdot \mathbf{B} \vec{\mathbf{n}} \vec{\mathbf{n}} \rangle = (\mathbf{L} - \langle \vec{\mathbf{n}} \vec{\mathbf{n}} \rangle : (\mathbf{L} - \mathbf{A}) \mathbf{I} + \mathbf{A}) \cdot \mathbf{B} \langle \vec{\mathbf{n}} \vec{\mathbf{n}} \rangle$$

and the definitions for the stress tensors $\sigma_s = \mathbf{A} \langle \vec{\mathbf{R}} \vec{\mathbf{R}} \rangle$ and $\sigma_c = \mathbf{B} \langle \vec{\mathbf{n}} \vec{\mathbf{n}} \rangle$, it follows:

$$\text{a) } \dot{\sigma}_s = (\mathbf{L} - \mathbf{A}) \cdot \sigma_s + \sigma_s \cdot (\mathbf{L} - \mathbf{A})^c \rightarrow \overset{\nabla}{\sigma}_s + \mathbf{A} \cdot \sigma_s + \sigma_s \cdot \mathbf{A}^c = 0$$

$$\text{b) } \dot{\sigma}_c = (\mathbf{L} - \hat{\mathbf{A}}_n) \cdot \sigma_c + \sigma_c \cdot (\mathbf{L} - \hat{\mathbf{A}}_n)^c \rightarrow \overset{\nabla}{\sigma}_c + \hat{\mathbf{A}}_n \cdot \sigma_c + \sigma_c \cdot \hat{\mathbf{A}}_n^c = 0$$

where:

$$\hat{\mathbf{A}}_n = \left(\frac{1}{\mathbf{B}} \sigma_c : (\mathbf{D} - \mathbf{A}) \mathbf{I} + \mathbf{A} \right)$$

A two mode model is obtained for which the slip tensor \mathbf{A} still has to be specified. These two modes are coupled if the slip tensor \mathbf{A} is a function the stress.

Example: Larsons constitutive equation

If \mathbf{A} is chosen as:

$$\mathbf{A} = \frac{\xi}{3G} (\sigma_c : \mathbf{D}) \mathbf{I}$$

then, using $B = 3\xi G$:

$$\hat{A}_n = \frac{1}{3\xi G}(\sigma_c:D) \mathbf{I} - \frac{1}{3\xi G}(\sigma_c:I) \frac{\xi}{3G}(\sigma_c:D) \mathbf{I} + \frac{\xi}{3G}(\sigma_c:D) \mathbf{I} = \frac{1}{3\xi G}(\sigma_c:D) \mathbf{I}$$

The following set of equations is obtained:

$$\text{a) } \dot{\sigma}_s + \frac{2}{3G}(\sigma_c:D) \sigma_s = 0$$

$$\text{b) } \dot{\sigma}_c + \frac{2}{3\xi G}(\sigma_c:D) \sigma_c = 0$$

These equations can be approximated by one constitutive equation in terms of the stress σ only.