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# Isothermal Implementation of the Eight-chain Model

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## Abstract

The eight-chain model [Arruda and Boyce, 1993a] is a hyperelastic model specifically developed for predicting the stress response of arbitrary large strain deformations of elastomeric materials. The eight-chain model, which requires three material parameters (a shear modulus, a bulk modulus and a locking stretch), is also used an important component in viscoplastic models for elastomers [Bergström and Boyce, 1998] and glassy polymers [Arruda and Boyce, 1993b].

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## 1 List of Symbols

Direct notation is used throughout, with the same conventions as in Truesdell and Noll [1965, 1992], Gurtin [1981] and Šilhavý [1997].

$\mathcal{B}_t \subset \mathbb{R}^3$       position of the material body  $\mathcal{B}$  at time  $t$

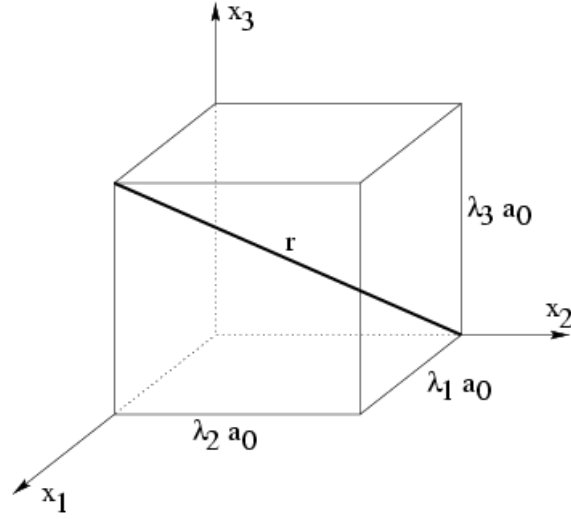
$\mathbf{p} \in \mathcal{B}_0$       position of a material point in the reference configuration

$\mathbf{x} \in \mathcal{B}_t$	position of a material point in the current configuration
$\mathbf{F} \in \text{Lin}^+$	deformation gradient
$\rho_0, \rho$	mass density in the reference and current configuration
$\mathbf{T}$	Cauchy stress
$e$	specific internal energy (i.e. per unit mass)
$\eta$	specific entropy
$\psi$	specific Helmholtz free energy
$W$	strain energy density (per unit reference volume)
$\theta$	absolute temperature

## 2 Constitutive Modeling of the Equilibrium Response of Elastomers

Consider an elastomeric body  $\mathcal{B}$  in its reference configuration  $\mathcal{B}_0 \subset \mathbb{R}^3$  with the corresponding material points labeled by  $\mathbf{p} \in \mathcal{B}_0$ . It is assumed that the boundary  $\partial\mathcal{B}_0$  of the region  $\mathcal{B}_0$  is regular enough to ensure the validity of the divergence theorem, and that the exterior normal  $\mathbf{n}_0$  to  $\mathcal{B}_0$  is defined for almost every point  $\mathbf{p}$  of  $\partial\mathcal{B}_0$ , where ‘almost everywhere’ means that the set of points where  $\mathbf{n}_0$  is not defined has the area measure zero. Denote by  $\chi_t(\mathbf{p}) : \mathcal{B}_0 \times \mathbb{R} \rightarrow \mathbb{R}^3$  a macroscopic motion of  $\mathcal{B}_0$  in a time interval  $t \in [0, t_1] \subset \mathbb{R}_+$  which maps any material point  $\mathbf{p}$  to the point  $\mathbf{x} = \chi_t(\mathbf{p}) \in \mathbb{R}^3$  in the deformed configuration  $\mathcal{B}_t = \chi_t(\mathcal{B}_0) \subset \mathbb{R}^3$ . In the following the reference configuration is taken to be stress-free with homogeneous reference temperature  $\theta_0 \in \mathbb{R}_+$ . The total deformation gradient defined by  $\mathbf{F} = \partial_{\mathbf{p}} \chi(\mathbf{p}, t)$  can be decomposed into distortional and dilatational parts:  $\mathbf{F} = (J)^{1/3} \mathbf{F}^*$  where  $J = \det(\mathbf{F})$ . To get a physical picture of the deformation process of an elastomer assume that the chain molecules can be considered to be located along the diagonals of a unit cell located in principal stretch space as illustrated in Figure 1 (this is the eight chain

assumption of Arruda and Boyce [1993a].) Denote the side lengths of the representative



**Figure 1:** Representative volume element used in the 8-chain model.

volume element in the reference state by  $a_0$  and the undeformed chain length by  $r_0$  (it then directly follows that  $r_0 = a_0\sqrt{3}$ .) Further take the macromolecules to be freely jointed with  $n$  rigid links each of length  $l$ . For this chain model the average end-to-end distance in the absence of an external force field is  $l\sqrt{n}$ . By defining  $\{\lambda_i^* | i = 1, \dots, 3\}$  to be the applied principal distortional stretches the effective distortional chain length becomes  $r = a_0[(\lambda_1^*)^2 + (\lambda_2^*)^2 + (\lambda_3^*)^2]^{1/2}$ , giving the effective distortional chain stretch

$$\bar{\lambda}^* = \left[ \frac{(\lambda_1^*)^2 + (\lambda_2^*)^2 + (\lambda_3^*)^2}{3} \right]^{1/2} = \sqrt{\frac{\text{tr } \mathbf{C}^*}{3}} = \sqrt{\frac{\text{tr } \mathbf{B}^*}{3}},$$

where  $\mathbf{B}^* = (J)^{-2/3}\mathbf{B}$ . Based on this physical model, an *eight-chain material* is defined as an isotropic thermoelastic material whose strain energy density  $W$  only depends on the two invariants  $\bar{\lambda}^*(\mathbf{B}^*) := [\text{tr}(\mathbf{B}^*)/3]^{1/2}$ ,  $J(\mathbf{F})$ , and the temperature  $\theta$ . By noting that the effective chain stretch is related to the first invariant of  $\mathbf{B}^*$  through  $\bar{\lambda}^* = [I_1(\mathbf{B}^*)/3]^{1/2}$  it follows that the strain energy density can be written  $\bar{W}(\bar{\lambda}^*, J, \theta)$ , or alternatively  $\hat{W}(I_{1^*}, J, \theta)$  where  $I_{1^*} := I_1(\mathbf{B}^*) = \text{tr}(\mathbf{B}^*)$ . The Cauchy stress for an eight-chain material can then be

obtained from the continuum mechanics expression

$$\mathbf{T} = \frac{2}{J} \left[ \hat{W}_{1^*} + \hat{W}_{2^*} I_{1^*} \right] \mathbf{B}^* - \frac{2}{J} \hat{W}_{2^*} (\mathbf{B}^*)^2 + \left[ \frac{\partial \hat{W}}{\partial J} - \frac{2I_{1^*}}{3J} \hat{W}_{1^*} - \frac{4I_{2^*}}{3J} \hat{W}_{2^*} \right] \mathbf{1}, \quad (1)$$

which in this case with no dependence on  $I_{2^*}$  can be simplified to

$$\mathbf{T} = \frac{2}{J} \hat{W}_{1^*} \text{dev}[\mathbf{B}^*] + \frac{\partial \hat{W}}{\partial J} \mathbf{1} \quad (2)$$

or when expressed in terms of the effective chain stretch  $\bar{\lambda}^*$

$$\mathbf{T} = \frac{1}{J} \frac{1}{3\bar{\lambda}^*} \frac{\partial \bar{W}}{\partial \bar{\lambda}^*} \text{dev}[\mathbf{B}^*] + \frac{\partial \bar{W}}{\partial J} \mathbf{1}. \quad (3)$$

To determine the strain energy density  $\bar{W}$  first use the experimental observation that the internal energy is not a function of the applied distortional stretch, i.e.  $e(J, \theta)$ . The specific heat at constant volume, defined by  $c_v = \partial e(J, \theta) / \partial \theta$ , can then be written

$$c_v(J, \theta) = \frac{\partial \psi(\bar{\lambda}^*, J, \theta)}{\partial \theta} + \eta(\bar{\lambda}^*, J, \theta) + \theta \frac{\partial \eta(\bar{\lambda}^*, J, \theta)}{\partial \theta}. \quad (4)$$

where the definition of the Helmholtz free energy  $\psi(\bar{\lambda}^*, J, \theta) = e(J, \theta) - \theta \eta(\bar{\lambda}^*, J, \theta)$  has been used. Since the first two terms of the right hand side of (4) have to cancel to satisfy the Clausius-Duhem inequality the specific heat becomes

$$c_v(J, \theta) = \theta \frac{\partial \eta(\bar{\lambda}^*, J, \theta)}{\partial \theta}. \quad (5)$$

Further assume that the material is almost incompressible and that the temperature does not vary too much such that  $c_v$ , to a first order approximation, can be taken to be a constant.

Equation (5) then yields

$$\psi(\bar{\lambda}^*, J, \theta) = c_v \theta (1 - \ln \theta) + e_1(J) - \theta \eta(\bar{\lambda}^*, J). \quad (6)$$

Assuming small volumetric deformations, the linearized relationship between the Cauchy stress  $\mathbf{T}$  and the volumetric deformation  $J$  is taken as

$$\frac{\partial \bar{W}}{\partial J} = \mathbf{T} \propto \kappa (J - 1) \mathbf{1} \quad (7)$$

giving  $e_1(J) = \kappa J (J/2 - 1) / \rho_0$  which when inserted into (6) gives

$$\bar{W}(\bar{\lambda}^*, J, \theta) = \rho_0 c_v \theta [1 - \ln \theta] + \kappa J [J/2 - 1] - \theta \rho_0 \eta(\bar{\lambda}^*). \quad (8)$$

Note that the dependence on  $J$  in  $\eta(\bar{\lambda}^*, J)$  has been neglected due to the the assumption of small volume change. The Cauchy stress can then be calculated from (3) giving

$$\mathbf{T} = \frac{-\theta}{3J\bar{\lambda}^*} \frac{d[\rho_0 \eta(\bar{\lambda}^*)]}{d\bar{\lambda}^*} \text{dev}[\mathbf{B}^*] + \kappa [J - 1] \mathbf{1}. \quad (9)$$

Now it only remains to determine how the entropy depends on the effective chain stretch.

From the chain rule

$$\frac{\partial[\rho_0 \eta(r(\bar{\lambda}^*))]}{\partial \bar{\lambda}^*} = \frac{\partial[\rho_0 \eta]}{\partial r} \frac{\partial r}{\partial \bar{\lambda}^*} = \frac{\partial[\rho_0 \eta]}{\partial r} \frac{1}{\frac{\partial}{\partial r} \left[ \frac{r}{l\sqrt{n}} \right]} = l\sqrt{n} \frac{\partial[\rho_0 \eta]}{\partial r}$$

it is clear that it is sufficient to determine how the entropy of a single macromolecule depends on its end-to-end distance. By assuming the molecules to be freely jointed with a fixed bond length the entropy can be determined from the statistical mechanics relation  $[\rho_0 \eta] \propto N k_B \ln \Omega(r)$  where  $\Omega(r)$  is the probability distribution of the end-to-end distance of the molecular chain and  $N$  is the number of chains per unit volume. [Flory \[1988\]](#) showed that

the probability distribution under these conditions can be written

$$\Omega(r) = \frac{1}{2\pi^2 r} \int_0^\infty q \sin(qr) \left[ \frac{\sin ql}{ql} \right]^n dq. \quad (10)$$

One approximation of (10) good for  $n \gg 1$  and  $r \approx n$  is the Langevin expression attributed to [Kuhn and Gr \$\ddot{u}\$ n \[1942\]](#):

$$\Omega(r) = \frac{A'}{l^3} \left[ \frac{\sinh \beta}{\beta} \right]^n \exp \left[ \frac{-\beta r}{l} \right] \quad (11)$$

where  $\beta = \mathcal{L}^{-1}(r/(nl))$  and  $\mathcal{L}(x) = \coth(x) - 1/x$  is the Langevin function. The inverse Langevin function  $\mathcal{L}^{-1}(x)$  can be approximated by [\[Bergstr \$\ddot{o}\$ m and Boyce, 1999\]](#):

$$\mathcal{L}^{-1}(x) \approx \begin{cases} 1.31446 \tan(1.58986x) + 0.91209x, & \text{if } |x| < 0.84136 \\ 1/(\text{sign}(x) - x), & \text{if } 0.84136 \leq |x| < 1. \end{cases} \quad (12)$$

In the limit  $n \rightarrow \infty$ , Equation (11) becomes a Gaussian distribution

$$\Omega(r) = \left[ \frac{3}{2\pi nl^3} \right]^{3/2} \exp \left[ \frac{-3r^2}{2nl^2} \right]. \quad (13)$$

It is easy to show that the change in entropy with chain length for the Langevin expression therefore can be written

$$\frac{\partial[\rho_0 \eta]}{\partial r} = \frac{\partial[Nk_B \ln \Omega(r)]}{\partial r} = \frac{-Nk_B}{l} \mathcal{L}^{-1} \left( \frac{r}{nl} \right),$$

and that the corresponding expression for Gaussian chains becomes

$$\frac{\partial[\rho_0 \eta]}{\partial r} = \frac{\partial[Nk \ln \Omega(r)]}{\partial r} = -\frac{3Nk_B r}{nl^2}.$$

Equation (9) can now be written

$$\mathbf{T} = \frac{Nk_B\theta}{3J} \frac{\lambda^{\text{lock}}}{\bar{\lambda}^*} \mathcal{L}^{-1}\left(\frac{\bar{\lambda}^*}{\lambda^{\text{lock}}}\right) \text{dev}[\mathbf{B}^*] + \kappa[J-1]\mathbf{1}, \quad (14)$$

where  $\lambda^{\text{lock}} := nl$ . For the special case of incompressible uniaxial deformation Equation (14) simplifies to

$$\sigma = \frac{Nk_B\theta}{3J} \frac{\lambda^{\text{lock}}}{\bar{\lambda}^*} \mathcal{L}^{-1}\left(\frac{\bar{\lambda}^*}{\lambda^{\text{lock}}}\right) \left[\lambda^2 - \frac{1}{\lambda}\right] \quad (15)$$

and for simple shear defined by  $\mathbf{F} = \mathbf{1} + \gamma\mathbf{e}_1 \otimes \mathbf{e}_2$  the shear stress is given by

$$T_{12} = \frac{Nk_B\theta}{3J} \frac{\lambda^{\text{lock}}}{\bar{\lambda}^*} \mathcal{L}^{-1}\left(\frac{\bar{\lambda}^*}{\lambda^{\text{lock}}}\right) \gamma \quad (16)$$

where  $\bar{\lambda}^* = \sqrt{1 + \gamma^2/3}$ . The initial shear modulus of the material is given by  $\mu_0 = \frac{\partial T_{12}}{\partial \gamma} \Big|_{\gamma=0}$  giving

$$\mu_0 = \frac{Nk_B\theta_0}{3} \lambda^{\text{lock}} \mathcal{L}^{-1}\left(\frac{1}{\lambda^{\text{lock}}}\right) \quad (17)$$

which when inserted in (14) gives the Cauchy stress as

$$\mathbf{T} = \frac{\theta}{\theta_0} \frac{\mu_0}{J\bar{\lambda}^*} \frac{\mathcal{L}^{-1}\left(\frac{\bar{\lambda}^*}{\lambda^{\text{lock}}}\right)}{\mathcal{L}^{-1}\left(\frac{1}{\lambda^{\text{lock}}}\right)} \text{dev}[\mathbf{B}^*] + \kappa[J-1]\mathbf{1}. \quad (18)$$

For the special case of uniaxial deformation the corresponding equation becomes

$$\sigma = \frac{\mu_0}{\bar{\lambda}^*} \frac{\mathcal{L}^{-1}\left(\frac{\bar{\lambda}^*}{\lambda^{\text{lock}}}\right)}{\mathcal{L}^{-1}\left(\frac{1}{\lambda^{\text{lock}}}\right)} \left[\lambda^2 - \frac{1}{\lambda}\right]. \quad (19)$$

The constitutive relationship for the case of Gaussian chains is directly obtained by replacing

the inverse Langevin function by the first term in its series expansion  $\mathcal{L}^{-1}(x) \approx 3x$ , giving

$$\mathbf{T} = \frac{\theta}{\theta_0} \frac{\mu_0}{J} \text{dev}[\mathbf{B}^*] + \kappa[J - 1]\mathbf{1}, \quad (20)$$

which is a compressible neo-Hookean model.

Based on the results presented above, the deviatoric portion of the strain energy density for the eight-chain model can be written:

$$W_{dev}(\bar{\lambda}^*; \mu_0, \lambda^{\text{lock}}) = 3\mu_0 \left\{ \bar{\lambda}^* \frac{\beta}{\beta_0} - 1 - \frac{\lambda^{\text{lock}}}{\beta_0} \ln \left[ \frac{\sinh \beta}{\sinh \beta_0} \frac{\beta_0}{\beta} \right] \right\}, \quad (21)$$

where  $\bar{\lambda}^*$  is the deviatoric chain stretch,  $\beta = \mathcal{L}^{-1}(\bar{\lambda}^*/\lambda^{\text{lock}})$ , and  $\beta_0 = \mathcal{L}^{-1}(1/\lambda^{\text{lock}})$ . This function fulfills the requirement that  $W_{dev}(1, \mu_0, \lambda^{\text{lock}}) = 0$ . The corresponding strain energy density for the case with Gaussian chains becomes:

$$W_{dev} = \frac{3\mu_0}{2} (\bar{\lambda}^{*2} - 1) = \frac{\mu_0}{2} (I_1^* - 3). \quad (22)$$

## 2.1 Determination of the Material Constants

One way to determine the material constants used in Eq. (18) is to test the material in uniaxial loading conditions. The experimentally determined Young's modulus  $E$  is then correlated to  $\mu_0$  by

$$\mu_0 = \frac{E}{3}. \quad (23)$$

The parameter  $\kappa$  is the bulk modulus, which if unknown can simply be chosen sufficiently large, say  $\kappa \approx 100\mu_0$ . Finally, from the stress-strain curve it is possible to estimate the strain  $\epsilon_\infty$  at which the stress goes to infinity. The limiting chain stretch can then be calculated from

$$\bar{\lambda}^* = \sqrt{\frac{1}{3} [e^{2\epsilon_\infty} + 2e^{-\epsilon_\infty}]}. \quad (24)$$



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