On Capability of a Class of Incompressible Rate-type Fluid Models to Fit Experimental Data for Asphalt

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Abstract. We consider a class of viscoelastic rate type models that in particular includes: (i) Oldroyd-B fluid model with three parameters, (ii) nonlinear fluid model derived in *Rajagopal K. R., Srinivasa A. R.* [2000] with three parameters, and (iii) nonlinear model with five parameters. We are interested in observing how well are these models capable to capture the experimental data for asphalt performed by J. Murali Krishnan, Indian Institute of Technology, Madras using dynamic shear rheometer. We find out that the model (i) is not able to capture the experimentally observed overshoot for the torque, while we obtain overshoots for the models (ii) and (iii). Also, there are very small significant differences in the results established for models (ii) and (iii).

Introduction

In this paper we look for a mathematical model that would be able to describe the behavior of asphalt. The asphalt is a very complicated geomaterial and no suitable model to describe its disparate behavior exists at this moment. Many details about this material can be found in *Krishnan J. M., Rajagopal K. R.* [2003]. We consider three different rate-type fluid models and we investigate how well are these models capable to capture experiment with overshoot performed by J. Murali Krishnan.

Experimental data

We start with describing the experiment with asphalt performed by J. Murali Krishnan at Indian Institute of Technology Madras, *Krishnan, J. M.* [2007]. The experiment was performed using a dynamic shear rheometer which consists of two circular plates. A spherical sample of asphalt is placed between the plates and is squeezed into a disc. The lower plate is fixed and does not move, the upper plate starts to rotate at $t = 0$ s with a constant angular velocity ω_0 and the corresponding torque is recorded for times $0\,\mathrm{s} \le t \le T = 15\,\mathrm{s}$. The data set consists of the following: The height of the specimen is $h = 1$ mm and is maintained during the measurement. The radius of the plate is $R = 4$ mm. The experiment is conducted at a temperature of 35 °C at three different angular velocities. The measured torque is plotted against time in Figure 1.

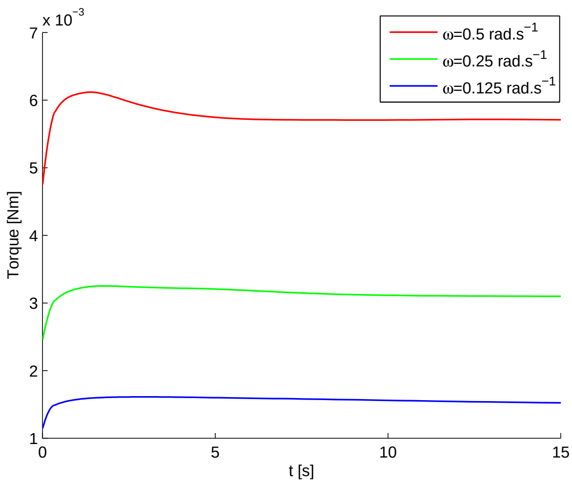

Figure 1. Experimental data: torque vs. time at constant temperature 35 °C.

Viscoelastic models

We are modeling the asphalt as an incompressible homogenous continuum with constant density ρ. Then the balance of mass reduces to

$$\operatorname{div} \mathbf{v} = 0, \tag{1}$$

where $\mathbf{v}$ is the velocity. Balance of linear momentum is given as

$$\rho \dot{\mathbf{v}} = \operatorname{div} \mathbf{T}, \tag{2}$$

and in the absence of internal couples, the balance of angular momentum implies that the stress tensor $\mathbf{T}$ is a symmetric tensor. Since we consider only isothermal processes, the balance of energy combined with the second law of thermodynamics reduces to the reduced thermodynamical inequality

$$0 \leq \xi = \mathbf{T} \cdot \mathbf{D} - \rho \dot{\psi}, \tag{3}$$

where ψ is the Helmholtz free energy and ξ is the rate of entropy production. These three balance equations and the reduced thermodynamical inequality have to be satisfied for all three viscoelastic models that we present in this paper. All considered models are the rate-type models, which means that the response between the stress tensor $\mathbf{T}$ and the symmetric part of the velocity gradient $\mathbf{D}$ is characterized through the differential equation. First we introduce the standard Oldroyd-B model, then two nonlinear models.

Oldroyd-B

Oldroyd-B is a standard linear model for viscoelastic fluids, *Oldroyd J. G.* [1950]. One of the possible way, how to derive this model, is the generalization of the model that we get by considering viscous fluid containing elastic springs with beads on its ends. The Oldroyd-B is in the following form

$$\begin{aligned} \mathbf{T} &= -p\mathbf{I} + 2\eta\mathbf{D} + G\mathbf{A}, \\ \mathbf{A} + \tau \overset{\triangledown}{\mathbf{A}} &= 2\tau\mathbf{D}, \end{aligned} \tag{4}$$

where the upper convected Oldroyd derivative is defined as

$$\overset{\triangledown}{\mathbf{A}} = \dot{\mathbf{A}} - \mathbf{L}\mathbf{A} - \mathbf{A}\mathbf{L}^{\mathrm{T}},$$

where $\mathbf{L} = \nabla \mathbf{v}$. This model contains three parameters: τ relaxation time, η viscosity and G shear modulus.

Nonlinear models

The nonlinear model was developed by *Rajagopal K. R., Srinivasa A. R.* [2000] using a framework for developing nonlinear models based on two notions: natural configuration and the principle of maximum entropy production.

The natural configuration $\kappa_{p(t)}$ is a configuration that the body occupying the current configuration κ_t attains on removal of external stimuli. More details about the concept of natural configuration can be found in *Rajagopal K. R., Srinivasa A. R.* [2004a]. Now we define some kinematics quantities and they are shown in Figure 2. The configuration κ_R denotes the reference (initial) configuration, the infinitesimal line is mapped from the reference into the current configuration κ_t through the deformation gradient $\mathbf{F}_{\kappa_\mathbf{R}}$. Infinitesimal line from the natural configuration $\kappa_{p(t)}$ that at time t corresponds to κ_t is mapped to infinitesimal line in κ_t through $\mathbf{F}_{\kappa_{p(t)}}$. Mapping $\mathbf{G}$ works between κ_R and $\kappa_{p(t)}$. The whole process is separated into purely elastic non-dissipative process $\mathbf{F}_{\kappa_{p(t)}}$ and the dissipative $\mathbf{G}$.

Using $\mathbf{F}_{\kappa_{p(t)}}$ we can define the left Cauchy-Green tensor, the rate of deformation and its symmetric part

$$\mathbf{B} = \mathbf{F}_{\kappa_{p(t)}} \mathbf{F}^{\mathrm{T}}_{\kappa_{p(t)}}, \quad \mathbf{L}_p = \dot{\mathbf{G}}\mathbf{G}^{-1}, \quad \mathbf{D}_p = \frac{1}{2}\left(\mathbf{L}_p + \mathbf{L}_p^{\mathrm{T}}\right).$$

Now one can compute the Oldroyd derivative of $\mathbf{B}$ and obtain

$$\overset{\triangledown}{\mathbf{B}} = -2\mathbf{F}_{\kappa_{p(t)}} \mathbf{D}_p \mathbf{F}^{\mathrm{T}}_{\kappa_{p(t)}}. \tag{5}$$

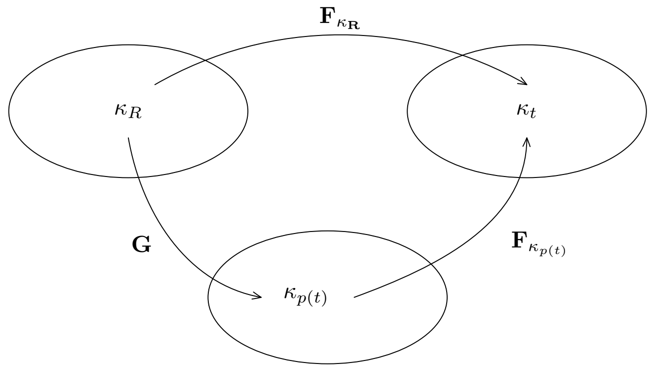

Figure 2. Natural configuration.

The derivation of the model in *Rajagopal K. R., Srinivasa A. R.* [2000] is based on specifying the constitutive equations for two scalar quantities, namely Helmholtz free energy ψ and the rate of entropy production ξ. Helmholtz free energy is described by the nonlinear neo-Hookean elastic response

$$\psi = \frac{\mu}{2\rho}\left(\operatorname{tr}\mathbf{B} - 3\right). \tag{6}$$

The rate of entropy production ξ indicates how the body dissipates energy

$$\xi = \epsilon_0(\mathbf{D}\cdot\mathbf{D}) + \epsilon_1(\mathbf{D}_p\cdot\mathbf{B}\mathbf{D}_p), \tag{7}$$

where $\epsilon_0, \epsilon_1 > 0$ in (7) are material coefficients. The first term in (7) represents the dissipation of Newtonian fluid, the second term corresponds to the dissipation due to interaction of viscous and elastic parts of fluid. Inserting (6) into the reduced thermodynamical inequality (3) we get

$$\xi = (\mathbf{T} - \mu\mathbf{B})\cdot\mathbf{D} + \mu\mathbf{B}\cdot\mathbf{D}_p.$$

Now, we use the principle of maximum rate of entropy production, more details can be found in *Rajagopal K. R., Srinivasa A. R.* [2004b]. So, we maximize $\xi(\mathbf{D}, \mathbf{D}_p)$ among the values of $\mathbf{D}$ and $\mathbf{D}_p$ fulfilling the constraints of incompressibility $\operatorname{tr}\mathbf{D} = \operatorname{tr}\mathbf{D}_p = 0$ and the reduced thermodynamical inequality (3). For this purpose we use the method of Lagrange multipliers and get

$$2\frac{1+\lambda_1}{\lambda_1}\epsilon_0\mathbf{D} = \mathbf{T} - \mu\mathbf{B} + \frac{\lambda_2}{\lambda_1}\mathbf{I},$$
$$2\frac{1+\lambda_1}{\lambda_1}\epsilon_1\mathbf{B}\mathbf{D}_p = \mu\mathbf{B} + \frac{\lambda_3}{\lambda_1}\mathbf{I},$$

where $\lambda_1, \lambda_2, \lambda_3$ are Lagrange multipliers. Using isotropy of neo-Hookean law, i.e. $\mathbf{F}_{\kappa_{p(t)}} = \mathbf{F}^{\mathrm{T}}_{\kappa_{p(t)}}$, doing some algebraic manipulations and using (5) we arrive to the nonlinear model with three parameters (for details see *Rajagopal K. R., Srinivasa A. R.* [2000]) that we summarize below.

Nonlinear model with three parameters

The stress tensor is in the form

$$\mathbf{T} = -p\mathbf{I} + \epsilon_0\mathbf{D} + \mu\mathbf{B},$$

where $\mathbf{B}$ satisfies the following differential equation

$$\overset{\triangledown}{\mathbf{B}} = -2\frac{\mu}{\epsilon_1}\left(\mathbf{B} - \lambda\mathbf{I}\right) \tag{8}$$

with

$$\lambda = \frac{3}{\operatorname{tr}\left(\mathbf{B}^{-1}\right)} = \frac{6\det\mathbf{B}}{\left(\operatorname{tr}\mathbf{B}\right)^2 - \operatorname{tr}\left(\mathbf{B}^2\right)} = \frac{6}{\left(\operatorname{tr}\mathbf{B}\right)^2 - \operatorname{tr}\left(\mathbf{B}^2\right)}.$$

The first equality is valid due to Cayley-Hamilton theorem, the other due to incompressibility. This model contains three parameters: ϵ_0, ϵ_1 are the viscous coefficients, μ is the elastic coefficient.

Nonlinear model with five parameters

In order to have a model that might be more suitable to describe the behavior of the asphalt, we modify the above derivation by considering the rate of entropy production ξ in the more general form, namely

$$\xi = \epsilon_0(\mathbf{D}\cdot\mathbf{D})^{\alpha} + \epsilon_1(\mathbf{D}_p\cdot\mathbf{B}\mathbf{D}_p)^{\beta}, \quad \alpha > 0,\ \beta > 0.5.$$

Proceeding as in derivation of nonlinear model with three parameters, we obtain

$$\mathbf{T} = -p\mathbf{I} + \alpha\chi\epsilon_0\left(\mathbf{D}\cdot\mathbf{D}\right)^{\alpha-1}\mathbf{D} + \mu\mathbf{B}$$

satisfying

$$\sqrt{\operatorname{tr}\mathbf{B} - 3\lambda}\ \overset{\triangledown}{\mathbf{B}} = -2(\mathbf{B} - \lambda\mathbf{I})\sqrt{X}, \tag{9}$$

where X is a solution of the algebraic equation

$$\beta^2\epsilon_1^2\chi^2X^{2\beta-1} = \mu^2\left(\operatorname{tr}\mathbf{B} - 3\lambda\right), \quad \chi = \frac{\frac{\epsilon_0}{\epsilon_1}\left(\mathbf{D}\cdot\mathbf{D}\right)^{\alpha} + X^{\beta}}{\alpha\frac{\epsilon_0}{\epsilon_1}\left(\mathbf{D}\cdot\mathbf{D}\right)^{\alpha} + \beta X^{\beta}}. \tag{10}$$

This model contains five parameters: ϵ_0, ϵ_1 viscous coefficients, μ elastic coefficient, $\alpha > 0, \beta > 0.5$. For $\alpha < 1$ this model provides shear thinning, for $\alpha > 1$ shear thickening, and for $\alpha = \beta = 1$ reduces to the previous model.

Simulation of the experiment

We simulate the experiment in the cylindrical coordinates r, φ, z because of the geometry of the experiment. The flow is axially symmetric, that is why all variables do not depend on φ. For simplicity we assume the velocity to be given by

$$\mathbf{v} = \left(0, \frac{\omega(t)rz}{h}, 0\right),$$

where $\omega(t) = H_0\omega$ and H_0 is the Heaviside Function. Furthermore we neglect the term $\frac{\partial\omega}{\partial t}$, $\omega(t) = \omega = const$. The initial conditions for the models are following (the material is relaxed at the beginning):

$$\begin{aligned} \mathbf{A}(t=0) &= \mathbf{0} \text{ for Oldroyd-B,} \\ \mathbf{B}(t=0) &= \mathbf{0} \text{ for nonlinear models.} \end{aligned} \tag{11}$$

After we solve the model, we compute the component of the stress tensor $T_{\varphi z}$, and from that we get by integrating the torque M on the upper plate

$$M(t) = \int_{\text{upper plate}} rT_{\varphi z}\,\mathrm{d}S = \int_0^R 2\pi r^2 T_{\varphi z}(r, z=h)\,\mathrm{d}r. \tag{12}$$

Oldroyd-B

Assume that the solution is in this form

$$p = p(t,r,z), \quad \mathbf{v} = \left(0, \frac{\omega rz}{h}, 0\right), \quad \mathbf{A} = \begin{pmatrix} A_{rr} & A_{r\varphi} & A_{rz} \\ A_{r\varphi} & A_{\varphi\varphi} & A_{\varphi z} \\ A_{rz} & A_{\varphi z} & A_{zz} \end{pmatrix}(t,r,z).$$

Substitute it into the governing equations (4) and using the simplification and the initial conditions (11), we get

$$\frac{\partial p}{\partial r} = -G\frac{A_{\varphi\varphi}}{r}, \qquad \frac{\partial p}{\partial z} = 0,$$

$$A_{rr} = A_{r\varphi} = A_{rz} = A_{zz} = 0, \qquad \frac{\partial A_{\varphi\varphi}}{\partial t} = -\frac{1}{\tau}A_{\varphi\varphi} + \frac{2r\omega}{h}A_{\varphi z},$$

$$\frac{\partial A_{\varphi z}}{\partial t} = -\frac{1}{\tau}A_{\varphi z} + \frac{r\omega}{h}.$$

Since we are interested in torque (12), we need to know $A_{\varphi z}$ to compute $T_{\varphi z}$. We have

$$A_{\varphi z} = \frac{\tau r \omega}{h}\left(1 - e^{-t/\tau}\right) \Rightarrow T_{\varphi z} = \frac{\omega r}{h}\left(\eta + \tau G(1 - e^{-t/\tau})\right) \Rightarrow M = \frac{\pi \omega R^4}{2h}\left(\eta + \tau G(1 - e^{-t/\tau})\right).$$

From this formula we can immediately see that this model is not able to capture the overshoot of the torque at the beginning of the experiment. The most convenient parameters τ, η, G are found using least square method (Matlab function `fit`). The result is in Figure 3. The maximum relative error is 3.6%, the average relative error is 2.8%. The maximum relative error $g_{\max}$ and average relative error g_{average} are computed as

$$g_{\max} = \max_{0 \le t \le T}\left|1 - \frac{M(t)}{E(t)}\right|, \quad g_{\text{average}} = \frac{1}{T}\int_0^T \left|1 - \frac{M(t)}{E(t)}\right|,$$

where $E(t)$ are the experimental data and $M(t)$ is the computed torque.

Nonlinear model with three parameters

Again assuming the solution in the following form

$$p = p(t, r, z), \quad \mathbf{v} = \left(0, \frac{\omega r z}{h}, 0\right), \quad \mathbf{B} = \begin{pmatrix} B_{rr} & B_{r\varphi} & B_{rz} \\ B_{r\varphi} & B_{\varphi\varphi} & B_{\varphi z} \\ B_{rz} & B_{\varphi z} & B_{zz} \end{pmatrix}(t, r, z) \tag{13}$$

and substituting into the governing equations (8) and using the simplification and the initial conditions (11), we get

$$\frac{\partial p}{\partial r} = \mu\left(\frac{\partial B_{zz}}{\partial r} + \frac{B_{zz}}{r} - \frac{B_{\varphi\varphi}}{r}\right), \qquad \frac{\partial p}{\partial z} = \mu \frac{\partial B_{zz}}{\partial z},$$

$$B_{r\varphi} = Brz = 0, \qquad B_{rr} = B_{zz},$$

$$\frac{\partial B_{\varphi\varphi}}{\partial t} = -\frac{2\mu}{\epsilon_1} B_{\varphi\varphi} + \frac{2r\omega}{h} B_{\varphi z} + \frac{2\mu}{\epsilon_1}\lambda, \qquad \frac{\partial B_{\varphi z}}{\partial t} = -\frac{2\mu}{\epsilon_1} B_{\varphi z} + \frac{r\omega}{h} B_{zz},$$

$$\frac{\partial B_{zz}}{\partial t} = -\frac{2\mu}{\epsilon_1} B_{zz} + \frac{2\mu}{\epsilon_1}\lambda, \qquad \lambda = \frac{3}{2B_{\varphi\varphi}B_{zz} - B_{\varphi z}^2 + B_{zz}^2}.$$

Since we are again interested in knowing $B_{\varphi z}$, we solve only the last four equations. These equations can not be solved analytically. First we substitute λ, then we get the set of three equations. We solve it using Runge-Kutta method of the fourth order (Matlab function `ode45`) and compute

$$T_{\varphi z}(\epsilon_0, \epsilon_1, \mu, r, t) = \epsilon_0 r\omega/(2h) + \mu B_{\varphi z}(\mu/\epsilon_1, r, t).$$

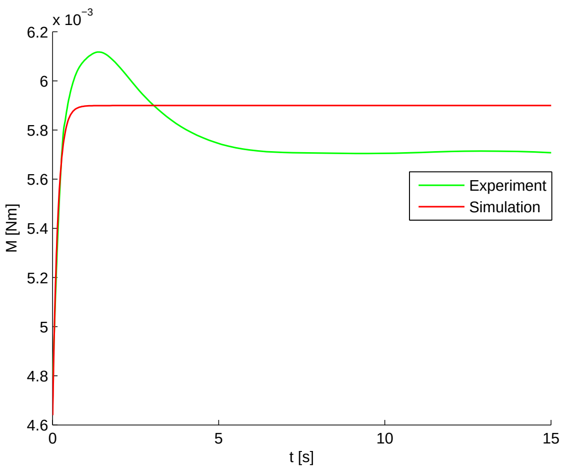

Figure 3. Fitting of Oldroyd-B at temperature 35 °C, $\omega = 0.5$ rad.s^{-1}.

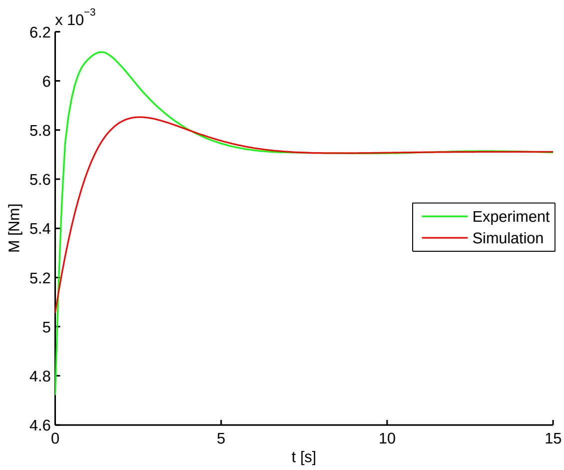

Figure 4. Fitting of the nonlinear model with three parameters at temperature 35 °C, $\omega = 0.5$ rad.s^{-1}.

Using the composite Simpson's rule in four nodes we integrate it and get the torque

$$M(\epsilon_0, \epsilon_1, \mu, t) = \int_0^R 2\pi r^2 T_{\varphi z}(\epsilon_0, \epsilon_1, \mu, r, t)\, \mathrm{d}r.$$

We introduce the scalar function

$$g(\epsilon_0, \epsilon_1, \mu) = \int_0^T |e(t) - M(\epsilon_0, \epsilon_1, \mu, t)|\, \mathrm{d}t$$

and find $\epsilon_0, \epsilon_1, \mu$, so that they minimize g (Matlab function `fminsearch`). The result is in the Figure 4. One can see that this model is better in capturing the overshoot of the torque at the beginning of the experiment, but still the result is not perfect. The maximum relative error is 8.7%, the average relative error is 1.1%.

Nonlinear model with five parameters

Again we assume the same form of solution as in the previous case (13) and substitute it into the governing equations (9), use the simplification and the initial conditions (11). Since we are interested in computing $B_{\varphi z}$, we need only the following seven equations

$$\frac{\partial B_{rr}}{\partial t} = -2\sqrt{X} B_{rr} + 2\sqrt{X}\lambda, \qquad \frac{\partial B_{r\varphi}}{\partial t} = -2\sqrt{X} B_{r\varphi} + \frac{r\omega}{h} B_{rz},$$
$$\frac{\partial B_{rz}}{\partial t} = -2\sqrt{X} B_{rz}, \qquad \frac{\partial B_{\varphi\varphi}}{\partial t} = -2\sqrt{X} B_{\varphi\varphi} + \frac{2r\omega}{h} B_{\varphi z} + 2\sqrt{X}\lambda,$$
$$\frac{\partial B_{\varphi z}}{\partial t} = -2\sqrt{X} B_{\varphi z} + \frac{r\omega}{h} B_{zz}, \qquad \frac{\partial B_{zz}}{\partial t} = -2\sqrt{X} B_{zz} + 2\sqrt{X}\lambda,$$

$$\lambda = \frac{3}{B_{\varphi\varphi} B_{zz} - B_{\varphi z}^2 - B_{rz}^2 + B_{rr} B_{zz} - B_{r\varphi}^2 + B_{rr} B_{\varphi\varphi}},$$

where X is the solution of (10) with $\mathbf{D} \cdot \mathbf{D} = \omega^2 r^2/(2h^2)$. We proceed similarly as in the previous case, but in addition at each time step we have to solve the algebraic equation (10). From the knowledge of the component $T_{\varphi z}$ we compute the torque on the upper plate and find the best parameters $\epsilon_0, \epsilon_1, \mu, \alpha, \beta$. The result is depicted in Figure 5. This model fits the experiment almost perfectly, the maximum relative error is 4.1%, and the average relative error is only 0.2%!

However, the above approach fits only one experiment. Since we would like to capture all three sets of experimental data (as drawn in Figure 1) with one set of parameters, we do the following test. We fit two experiments with the angular velocities $\omega = 0.25$ rad.s^{-1} and $\omega = 0.125$ rad.s^{-1} which results in finding five model parameters. Then with these five parameters we aim to fit the experimental data for $\omega = 0.5$ rad.s^{-1}. To do this we employ new scalar function g as a relative error of the experiment

$$g = (g_1^2 + g_2^2)^{1/2}, \quad g_i = \left(\int_0^T \left| 1 - \frac{M_i(t)}{E_i(t)} \right|^2 \right)^{1/2},$$

where g_1 and g_2 are the relative errors of each experiments, g is the global relative error. The result is in the Figure 6. The average relative error of two fitted experiments is 1.6%, the average relative error of the predicted experiment is 9.9%. If we do the test with the nonlinear model with three parameters (8) we get almost the same result.

Conclusion

We found out that these two nonlinear models (8) and (9) seem to describe the response of asphalt better than the Oldroyd-B model. We also found that though model (9) has as many as five material parameters compared to three in the case of model (8), their predictive capability for the class of experiments, that we are trying to describe, is nearly the same.

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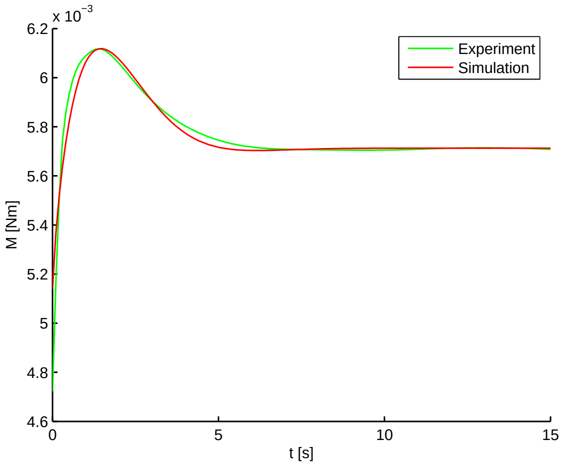

Figure 5. Fitting of the nonlinear model with five parameters at temperature 35 °C, $\omega = 0.5$ rad.s^{-1}.

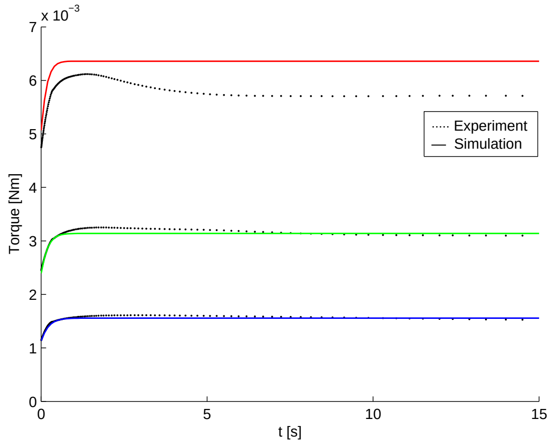

Figure 6. Predicting of the experiment for 35 °C, $\omega = 0.5$ rad.s^{-1}.

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