A new class of thermodynamically compatible viscoelastic models: Application and computational simulation

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Incompressible thermodynamically compatible viscoelastic model

Balance equations:

$$\operatorname{div} \mathbf{v} = 0,$$
$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = \operatorname{div} \mathbf{T}, \mathbf{T} = \mathbf{T}^{\mathrm{T}}.$$

Relation for Cauchy stress tensor $\mathbf{T}$ has to be added.

$$\mathbf{T} = -p\mathbf{I} + \mathbf{S},$$

rate-type fluid models – $\mathbf{S}$ satisfies evolutionary equation

Standard viscoelastic rate-type fluid models

Cauchy stress tensor in the form $\mathbf{T} = -p\mathbf{I} + \mathbf{S}$

Maxwell

$$\mathbf{S} = G(\mathbf{B} - \mathbf{I}),$$

$$\mathbf{S} + \tau \overset{\triangledown}{\mathbf{S}} = \mu \mathbf{D} \qquad \overset{\triangledown}{\mathbf{B}} + \frac{1}{\tau}(\mathbf{B} - \mathbf{I}) = \mathbf{0}, \quad \tau = \frac{\mu}{G}.$$

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

Oldroyd-B

$$\mathbf{S} = 2\mu_2 \mathbf{D} + \mathbf{A} \qquad \mathbf{S} = 2\mu_2 \mathbf{D} + G(\mathbf{B} - \mathbf{I}),$$

$$\mathbf{A} + \tau \overset{\triangledown}{\mathbf{A}} = \mu_1 \mathbf{D} \qquad \overset{\triangledown}{\mathbf{B}} + \frac{1}{\tau}(\mathbf{B} - \mathbf{I}) = \mathbf{0}, \quad \tau = \frac{\mu_1}{G}.$$

Burgers

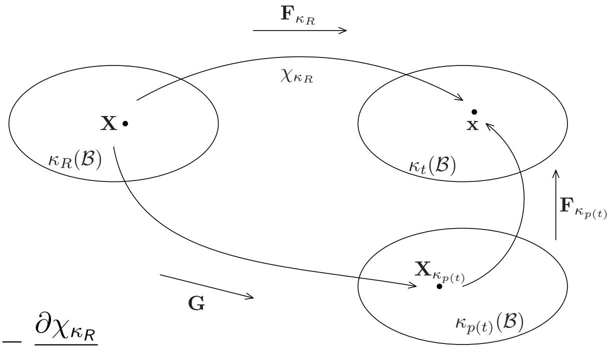
$$\mathbf{S} + \lambda_1 \overset{\triangledown}{\mathbf{S}} + \lambda_2 \overset{\triangledown\triangledown}{\mathbf{S}} = \eta_1 \mathbf{D} + \eta_2 \overset{\triangledown}{\mathbf{D}}$$

Thermodynamical framework for derivation of viscoelastic models

- Rajagopal and Srinivasa (2000), second law of thermodynamics automatically satisfied
- thermodynamically compatible non-linear viscoelastic rate-type fluid model
- derivation of model by Rajagopal and Srinivasa (2000) was modified
- capable of capturing experimental data of viscoelastic fluids
- models reduce to standard Oldroyd-B and Burgers' models

Natural configuration

Using natural configuration the deformation is split into purely elastic and dissipative part.



$$\mathbf{F}_{\kappa_R} = \frac{\partial \chi_{\kappa_R}}{\partial X}$$

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

$$\dot{\mathbf{B}}_{\kappa_{p(t)}} = \mathbf{L}\mathbf{B}_{\kappa_{p(t)}} + \mathbf{B}_{\kappa_{p(t)}}\mathbf{L}^{\mathrm{T}} - 2\mathbf{F}_{\kappa_{p(t)}}\mathbf{D}_{\kappa_{p(t)}}\mathbf{F}_{\kappa_{p(t)}}^{\mathrm{T}}$$

Two constitutive relations for scalars are prescribed: thermodynamic potential (internal energy e, free energy ψ) and rate of entropy production ξ.

Internal energy e – neo-Hookean

$$e = e_0(\eta, \rho) + \frac{G}{2\rho}\left(\operatorname{tr}\mathbf{B}_{\kappa_{p(t)}} - 3\right)$$

Rate of entropy production ξ

$$0 \leq \tilde{\xi} = 2\mu_2|\mathbf{D}|^2 + 2\mu_1|\mathbf{D}_{\kappa_{p(t)}}|^2.$$

Rajagopal, Srinivasa (2000) used

$$0 \leq \tilde{\xi} = 2\mu_1\mathbf{D}_{\kappa_{p(t)}} \cdot \mathbf{B}_{\kappa_{p(t)}}\mathbf{D}_{\kappa_{p(t)}}.$$

The principle of maximization of rate of entropy production is used, it determines the manner in which the natural configuration evolve.

Two natural configurations can be used – every corresponds to one relaxation mechanism

Quadratic model with one natural configuration

$$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{D} + G\mathbf{B}^d_{\kappa_{p(t)}},\ \mathbf{B}^d_{\kappa_{p(t)}} = \mathbf{B}_{\kappa_{p(t)}} - \frac{1}{3}\left(\operatorname{tr}\mathbf{B}_{\kappa_{p(t)}}\right)\mathbf{I},$$

$$\overset{\triangledown}{\mathbf{B}}_{\kappa_{p(t)}} + \frac{1}{\tau}\mathbf{B}_{\kappa_{p(t)}}\mathbf{B}^d_{\kappa_{p(t)}} = \mathbf{0}.$$

Quadratic model with two natural configurations

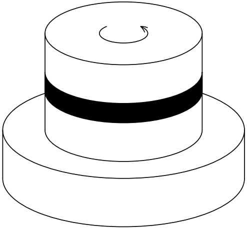
$$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{D} + G_1\mathbf{B}^d_{\kappa_{p_1(t)}} + G_2\mathbf{B}^d_{\kappa_{p_2(t)}},$$

$$\overset{\triangledown}{\mathbf{B}}_{\kappa_{p_1(t)}} + \frac{1}{\tau_1}\mathbf{B}_{\kappa_{p_1(t)}}\mathbf{B}^d_{\kappa_{p_1(t)}} = \mathbf{0},$$

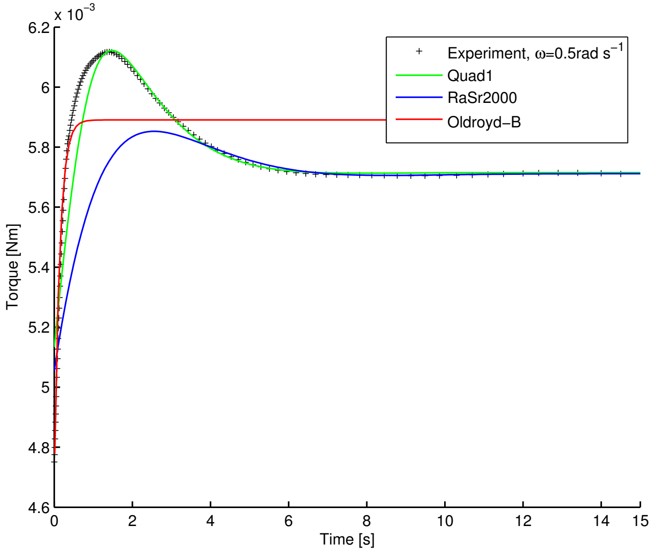
$$\overset{\triangledown}{\mathbf{B}}_{\kappa_{p_2(t)}} + \frac{1}{\tau_2}\mathbf{B}_{\kappa_{p_2(t)}}\mathbf{B}^d_{\kappa_{p_2(t)}} = \mathbf{0}.$$

Experiment Krishnan, Narayan (2007)

- torsional rheometer, height $h = 1$ mm, radius $R = 4$ mm
- upper plate rotates with constant angular velocity ω
- corresponding torque M is measured

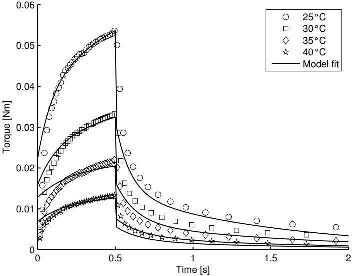


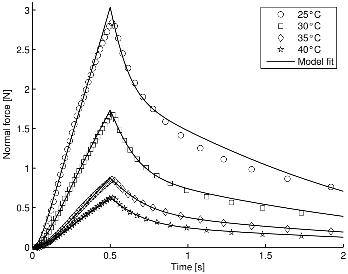
This experiment is fitted in cylindrical coordinates under the assumption that $\mathbf{v} = (0, \omega rz/h, 0)$.



$$\omega = \begin{cases} 0.5\text{rad s}^{-1} & 0\text{s} \leq t \leq 0.5\text{s} \\ 0\text{rad s}^{-1} & 0.5\text{s} < t \leq 2.0\text{s}. \end{cases}$$

corresponding torque and normal force are measured





Quadratic model with two natural configurations

$$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{D} + G_1\mathbf{B}^d_{\kappa_{p_1(t)}} + G_2\mathbf{B}^d_{\kappa_{p_2(t)}}$$

$$\overset{\triangledown}{\mathbf{B}}_{\kappa_{p_i(t)}} + \frac{1}{\tau_i}\mathbf{B}_{\kappa_{p_i(t)}}\mathbf{B}^d_{\kappa_{p_i(t)}} = \mathbf{0}, \quad i = 1, 2. \tag{1}$$

- model Quad2 capable of capturing experiments, where two different relaxation times are observed
- it linearizes to standard Burgers' model
- it can be shown that $\det \mathbf{B}_{\kappa_{p_i(t)}} = 1$ and $\operatorname{tr} \mathbf{B}_{\kappa_{p_i(t)}} \geq d$ where d is space dimension
- Quad2 used for the full simulations using FEM, based on the weak formulation, we obtain apriori estimates:
  multiply balance of linear momentum by $\mathbf{v}$, integrate over Ω, use Gauss theorem and summing with the traces of (1) and integrating over Ω

we get the following apriori estimates

$$\|\mathbf{v}\|_V \le C, \quad \|\mathbf{B}_{\kappa_{p_i(t)}}\|_{V_B} \le C, i = 1, 2, \tag{2}$$

where $V = L^\infty(0, T; L^2(\Omega))^d \cap L^2(0, T; W^{1,2}(\Omega))^d$,
$V_B = L^\infty(0, T; L^1(\Omega))^{d\times d} \cap L^2(0, T; L^2(\Omega))^{d\times d}$.
The following weak formulation is used

$$\int_\Omega \mathrm{tr}(\nabla \mathbf{v}) q \,\mathrm{d}x = 0,$$

$$\int_\Omega \rho \left[\frac{\partial \mathbf{v}}{\partial t} + (\nabla \mathbf{v})\mathbf{v}\right] \cdot \mathbf{q} \,\mathrm{d}x - \int_\Omega \mathbf{T} \cdot \nabla \mathbf{q} \,\mathrm{d}x + \int_{\Gamma_N} \mathbf{T}\mathbf{n} \cdot \mathbf{q} \,\mathrm{d}S = 0,$$

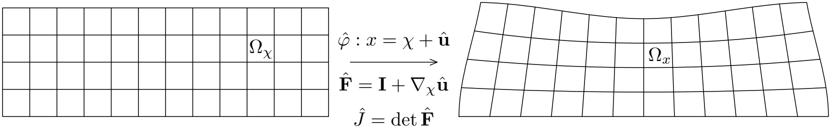
$$\mathbf{T} = -p\mathbf{I} + \mu\left((\nabla \mathbf{v}) + (\nabla \mathbf{v})^{\mathrm{T}}\right) + G_1 \mathbf{B}^d_{\kappa_{p_1(t)}} + G_2 \mathbf{B}^d_{\kappa_{p_2(t)}},$$

$$\int_\Omega \left[\frac{\partial \mathbf{B}_{\kappa_{p_1(t)}}}{\partial t} + (\nabla \mathbf{B}_{\kappa_{p_1(t)}})\mathbf{v} - (\nabla \mathbf{v})\mathbf{B}_{\kappa_{p_1(t)}} - \mathbf{B}_{\kappa_{p_1(t)}}(\nabla \mathbf{v})^{\mathrm{T}} + \frac{1}{\tau_1}\mathbf{B}_{\kappa_{p_1(t)}}\mathbf{B}^d_{\kappa_{p_1(t)}}\right] \cdot \mathbf{Q}_1 \,\mathrm{d}x = 0,$$

$$\int_\Omega \left[\frac{\partial \mathbf{B}_{\kappa_{p_2(t)}}}{\partial t} + (\nabla \mathbf{B}_{\kappa_{p_2(t)}})\mathbf{v} - (\nabla \mathbf{v})\mathbf{B}_{\kappa_{p_2(t)}} - \mathbf{B}_{\kappa_{p_2(t)}}(\nabla \mathbf{v})^{\mathrm{T}} + \frac{1}{\tau_2}\mathbf{B}_{\kappa_{p_2(t)}}\mathbf{B}^d_{\kappa_{p_2(t)}}\right] \cdot \mathbf{Q}_2 \,\mathrm{d}x = 0.$$

Full simulation in deforming domains

- problem computed on a fixed mesh $\Rightarrow$ the weak formulation transformed by $\hat{\varphi}$ from the physical domain in Ω_x to computational domain Ω_χ using arbitrary Langrangian-Eulerian description

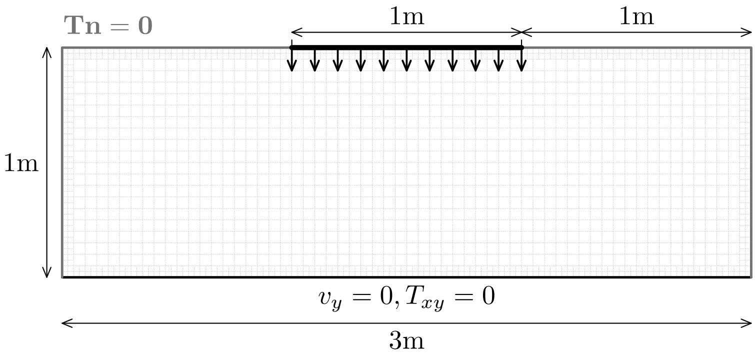


- new variable $\hat{\mathbf{u}}$ – arbitrary deformation of the domain and the mesh, $d\hat{\mathbf{u}}/dt = \mathbf{v}$ means material point
- monolithic approach is used and the problem is solved as one big coupled system of equations including the deformation of the mesh

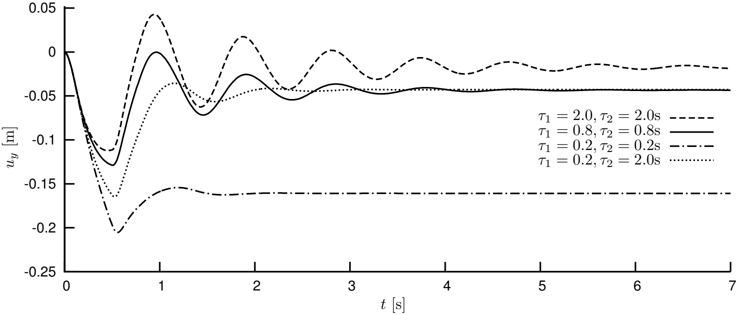
- discretization in time using conditionally stable ("almost" 3^{rd} order) Glowinski time scheme $\Delta t = 0.01$s
- discretization in space, regular square mesh, refined near boundary
- pressure p / velocity $\mathbf{v}$ / deformation $\mathbf{u}$ / parts of the stress $\mathbf{B}_{\kappa_{p_1(t)}}$ and $\mathbf{B}_{\kappa_{p_2(t)}}$ approximated by $\mathrm{P}_1^{\mathrm{disc}}$ / Q_2 / Q_2 / Q_2 / Q_2 elements
- monolithic solver, 45 DOFs / element
- Newton method & UMFPACK
- based on J. Hron's code

Pressing of viscoelastic material

- rectangular piece of material, width 3m, height 1m
- material is on the ground: it can fully slip in the x-direction, but it can not flow in the y-direction
- all other sides of the rectangle are free
- at $t = 0$ the material is at rest, and it is suddenly pushed in the middle at the top with a constant normal stress Tyy = -5 kPa for $\Delta t = 0.5$ s

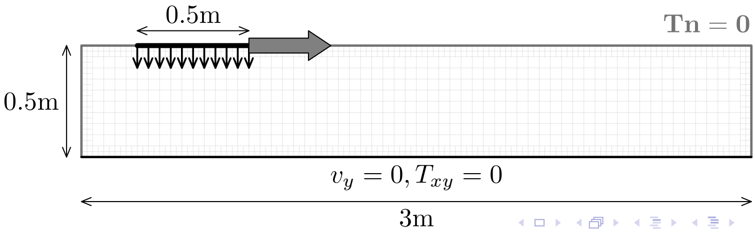


ρ [kg/m^3]	G_1 [kPa]	G_2 [kPa]	τ_1 [s]	τ_2 [s]	μ [Pa s]
1000	10	5	0.2	0.2	100
1000	10	5	0.2	2.0	100
1000	10	5	0.8	0.8	100
1000	10	5	2.0	2.0	100

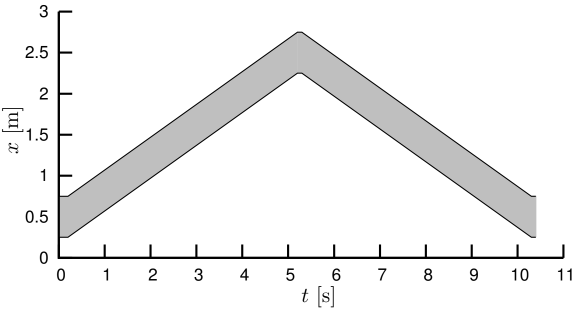


Rolling of the asphalt

- rectangular piece of material, width 3m, height 0.5m
- material is on the ground: it can fully slip in the x-direction, but it can not flow in the y-direction
- all other sides of the rectangle are free
- at $t = 0$ the material is at rest, and it is suddenly pushed at the top with a constant normal stress Tyy = -50 kPa
- force is applied on constant area $l = 50$cm corresponding to the weight $m = 2\,500$ kg and this area moves with the velocity 40 cm/s from the left to the right and then back to the left, i.e. the asphalt is rolled forward and back.
- force is released at $t = 10.4$ s and the material is let to relax



The location of the area where the force is applied w.r.t. time



Computed with two different set of parameters

	ρ [kg/m^3]	G_1 [kPa]	G_2 [kPa]	τ_1 [s]	τ_2 [s]	μ [Pa s]
edu	1000	10.000	5.000	0.200	2.000	10
real	1200	130.426	27.720	0.168	1.498	45 313