An introduction to implicit constitutive theory to describe the response of bodies

Vít Průša
prusv@karlin.mff.cuni.cz

Mathematical Institute, Charles University in Prague

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Balance laws, Navier–Stokes fluid, non-Newtonian fluids

Physical laws:

$$\rho \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \operatorname{div} \mathbf{T} + \rho \mathbf{b}$$
$$\operatorname{div} \mathbf{v} = 0$$
$$\mathbf{T} = \mathbf{T}^\top$$

Material properties:

$$\mathbf{T} = \mathbf{T}(\mathbf{v}, \nabla \mathbf{v}, \dots)$$

Navier–Stokes fluid:

$$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{D}$$

Non-newtonian fluids:

$$\mathbf{T} \neq -p\mathbf{I} + 2\mu\mathbf{D}$$

(a) Weissenberg effect.

(b) Barus effect.

Figure: Some non-newtonian effects.

Non-newtonian fluids: molten chocolate, polymer melts, ball point pen ink, aqueous limestone suspension, toothpaste, mineral oils, paints, mango jam, asphalt binder, blood

"Shear rate" dependent viscosity, $\mu = \mu(\mathbf{D})$

$$\mathbf{T} = -p\mathbf{I} + 2\mu(\mathbf{D})\mathbf{D}$$

$$\mu(\mathbf{D}) = \mu_\infty + \frac{\mu_0 - \mu_\infty}{\left(1 + \alpha \left|\mathbf{D}\right|^2\right)^{\frac{n}{2}}}$$

$$\mu(\mathbf{D}) = \mu_\infty + \left(\mu_0 - \mu_\infty\right)\left(1 + \alpha \left|\mathbf{D}\right|^a\right)^{\frac{n-1}{a}}$$

Pierre J. Carreau. Rheological equations from molecular network theories. *J. Rheol.*, 16(1):99–127, 1972

Kenji Yasuda. *Investigation of the analogies between viscometric and linear viscoelastic properties of polystyrene fluids*. PhD thesis, Massachusetts Institute of Technology. Dept. of Chemical Engineering., 1979

Differential type models

$$\mathbf{T} = -p\mathbf{I} + \mathfrak{f}(\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3, \dots)$$

$$\begin{aligned}
\mathbf{A}_1 &=_{\mathrm{def}} 2\mathbf{D} \\
\mathbf{A}_n &=_{\mathrm{def}} \frac{\mathrm{d}\mathbf{A}_{n-1}}{\mathrm{d}t} + \mathbf{A}_{n-1}\mathbf{L} + \mathbf{L}^{\top}\mathbf{A}_{n-1}
\end{aligned}$$

R. S. Rivlin and J. L. Ericksen. Stress-deformation relations for isotropic materials. *J. Ration. Mech. Anal.*, 4:323–425, 1955:

Incompressible simple fluid

$$\mathbf{T} = -p\mathbf{I} + 2\mu(\mathbf{D})\mathbf{D}$$
$$\mathbf{T} = -p\mathbf{I} + \mathfrak{f}(\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3, \dots)$$

General constitutive relation:

$$\mathbf{T} = -p\mathbf{I} + \mathfrak{F}_{s=0}^{+\infty}(\mathbf{C}_t\,(t-s))$$

C. Truesdell and W. Noll. The non-linear field theories of mechanics. In S. Flüge, editor, *Handbuch der Physik*, volume III/3. Springer, Berlin-Heidelberg-New York, 1965

Rate type models

$$\mathbf{T} = -\pi \mathbf{I} + \mathbf{S}$$

J. G. Oldroyd. Non-newtonian effects in steady motion of some idealized elastico-viscous liquids. *Proc. R. Soc. A-Math. Phys. Eng. Sci.*, 245(1241):278–297, 1958:

$$\mathbf{S} + \lambda_1 \overset{\triangledown}{\mathbf{S}} + \frac{\lambda_3}{2}\left(\mathbf{D}\mathbf{S} + \mathbf{S}\mathbf{D}\right) + \frac{\lambda_5}{2}\left(\operatorname{Tr}\mathbf{S}\right)\mathbf{D} + \frac{\lambda_6}{2}\left(\mathbf{S} \cdot \mathbf{D}\right)\mathbf{I} = -\mu\left(\mathbf{D} + \lambda_2 \overset{\triangledown}{\mathbf{D}} + \lambda_4 \mathbf{D}^2 + \frac{\lambda_7}{2}\left(\mathbf{D} \cdot \mathbf{D}\right)\mathbf{I}\right)$$

$$\overset{\triangledown}{\mathbf{b}} =_{\mathrm{def}} \frac{\mathrm{d}\mathbf{b}}{\mathrm{d}t} - \left[\nabla \mathbf{v}\right]\mathbf{b} - \mathbf{b}\left[\nabla \mathbf{v}\right]^{\top}$$

Pressure dependent viscosity, $\mu = \mu(p)$

$$
\begin{aligned}
\mathbf{T} &= -p\mathbf{I} + 2\mu(p)\mathbf{D} \\
\mu(p) &= \mu_0 \mathrm{e}^{\alpha p}
\end{aligned}
$$

P. W. Bridgman. The effect of pressure on the viscosity of forty-four pure liquids. *Proc. Am. Acad. Art. Sci.*, 61(3/12):57–99, FEB-NOV 1926

Stress dependent viscosity, $\mu = \mu(\mathbf{T})$

Gilbert R. Seely. Non-newtonian viscosity of polybutadiene solutions. *AIChE J.*, 10(1):56–60, 1964:

$$\mu(\mathbf{T}) = \mu_\infty + (\mu_0 - \mu_\infty)\,\mathrm{e}^{-\frac{|\mathbf{T}_\delta|}{\tau_0}}$$

H Blatter. Velocity and stress-fields in grounded glaciers – a simple algorithm for including deviatoric stress gradients. *J. Glaciol.*, 41(138):333–344, 1995:

$$\mu(\mathbf{T}) = \frac{A}{\left(|\mathbf{T}_\delta|^2 + \tau_0^2\right)^{\frac{n-1}{2}}}$$

Seikichi Matsuhisa and R. Byron Bird. Analytical and numerical solutions for laminar flow of the non-Newtonian Ellis fluid. *AIChE J.*, 11(4):588–595, 1965:

$$\mu(\mathbf{T}) = \frac{\mu_0}{1 + \alpha\,|\mathbf{T}_\delta|^{n-1}}$$

Implicit relation between $\mathbf{T}$ and $\mathbf{D}$

Constitutive relations have the form

$$\mathbf{T} = -p\mathbf{I} + 2\mu(\mathbf{D})\mathbf{D}$$
$$\mathbf{T} = -p\mathbf{I} + 2\mu(\mathbf{T})\mathbf{D}$$

or

$$\mathbf{T} = -p\mathbf{I} + \mathbf{S}$$
$$\mathfrak{f}(\mathbf{S}, \overset{\triangledown}{\mathbf{S}}, \dots, \mathbf{D}, \overset{\triangledown}{\mathbf{D}}, \dots) = \mathbf{0}$$

Incompressibility:

$$\operatorname{Tr}\mathbf{T} = -3p$$

General constitutive relation:

$$\mathbf{T} = -p\mathbf{I} + \mathfrak{F}_{s=0}^{+\infty}(\mathbf{C}_t\,(t-s))$$

Implicit constitutive relations

Relations of type

$$\mathfrak{f}\left(\mathbf{T},\mathbf{D}\right)=\mathbf{0}$$

or

$$\mathfrak{H}_{s=0}^{+\infty}\left(\mathbf{T}(t-s),\mathbf{C}_{t}\left(t-s\right)\right)=\mathbf{0}$$

allow one to bring under one unifying theme a much richer and wider class of material response.

A. J. A. Morgan. Some properties of media defined by constitutive equations in implicit form. *Int. J. Eng. Sci.*, 4(2):155–178, 1966

K. R. Rajagopal. On implicit constitutive theories. *Appl. Math., Praha*, 48(4):279–319, 2003

K. R. Rajagopal. On implicit constitutive theories for fluids. *J. Fluid Mech.*, 550:243–249, 2006

Stress power law models

Classical power-law fluids:

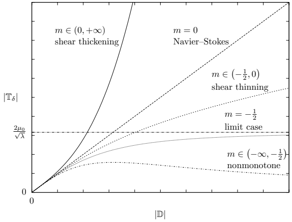
$$\mathbf{T} = -p\mathbf{I} + 2\mu_0 \left(1 + |\mathbf{D}|^2\right)^m \mathbf{D}$$

Stress power-law fluids:

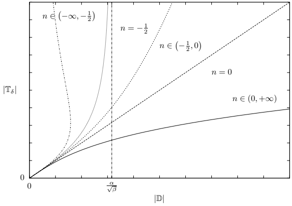
$$\mathbf{D} = \alpha \left(1 + \beta\, |\mathbf{T}_\delta|^2\right)^n \mathbf{T}_\delta$$

J. Málek, V. P., and K. R. Rajagopal. Generalizations of the Navier–Stokes fluid from a new perspective. *Int. J. Eng. Sci.*, 48(12):1907–1924, 2010

Qualitative behaviour



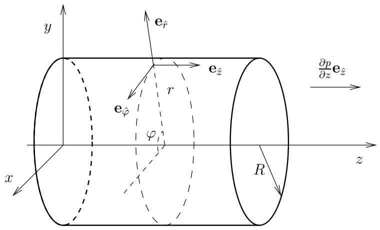
(a) Classical power-law model.



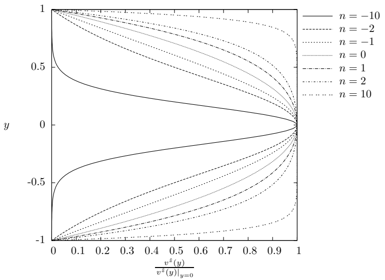
(b) Stress power law model.

Figure: Comparison of stress power-law model and the classical power law model.

Analytical solutions – Hagen–Poiseuille flow



(a) Geometry.



(b) Analytical solution.

Figure: Hagen–Poiseuille flow.

$$v^{\hat{z}}(r) = -\frac{1}{2\mathcal{R}(n+1)}\left(\left(1 + 2\mathcal{R}r^2\right)^{n+1} - (1 + 2\mathcal{R})^{n+1}\right).$$

Fully implicit models

Algebraic type relations:

$$\mathfrak{f}(\mathbf{T}, \mathbf{D}) = \mathbf{0}$$

General relation for isotropic tensor function of **T** and **D**:

$$\begin{aligned} &\alpha_0 \mathbf{I} + \alpha_1 \mathbf{T} + \alpha_2 \mathbf{D} + \alpha_3 \mathbf{T}^2 + \alpha_4 \mathbf{D}^2 + \alpha_5 (\mathbf{T}\mathbf{D} + \mathbf{D}\mathbf{T}) \\ &+ \alpha_6 \left(\mathbf{T}^2\mathbf{D} + \mathbf{D}\mathbf{T}^2\right) + \alpha_7 \left(\mathbf{T}\mathbf{D}^2 + \mathbf{D}^2\mathbf{T}\right) + \alpha_8 \left(\mathbf{T}^2\mathbf{D}^2 + \mathbf{D}^2\mathbf{T}^2\right) = \mathbf{0}, \end{aligned}$$

$$\begin{aligned} \alpha_i = \alpha_i \big(&\operatorname{Tr}\mathbf{D}, \operatorname{Tr}\mathbf{T}, \operatorname{Tr}\mathbf{D}^2, \operatorname{Tr}\mathbf{T}^2, \operatorname{Tr}\mathbf{T}^3, \operatorname{Tr}\mathbf{D}^2, \\ &\operatorname{Tr}(\mathbf{T}\mathbf{D}), \operatorname{Tr}\left(\mathbf{T}^2\mathbf{D}\right), \operatorname{Tr}\left(\mathbf{T}\mathbf{D}^2\right), \operatorname{Tr}\left(\mathbf{T}^2\mathbf{D}^2\right)\big) \end{aligned}$$

Fading memory

Explicit formula for Cauchy stress:

$$\mathbf{T} = -p\mathbf{I} + \mathfrak{F}_{s=0}^{+\infty}(\mathbf{C}_t\,(t-s))$$

Bernard D. Coleman and Walter Noll. An approximation theorem for functionals, with applications in continuum mechanics. *Arch. Ration. Mech. Anal.*, 6:355–370, 1960

Implicit relation between the histories:

$$\mathfrak{H}_{s=0}^{+\infty}\left(\mathbf{T}(t-s), \mathbf{C}_t\,(t-s)\right) = \mathbf{0}$$

V. P. and K. R. Rajagopal. On implicit constitutive relations for materials with fading memory. *J. Non-Newton. Fluid Mech.*, 2012. Accepted for publication

Rate type models

$$\mathbf{T} = -\pi \mathbf{I} + \mathbf{S}$$

J. G. Oldroyd. Non-newtonian effects in steady motion of some idealized elastico-viscous liquids. *Proc. R. Soc. A-Math. Phys. Eng. Sci.*, 245(1241):278–297, 1958:

$$\mathbf{S} + \lambda_1 \overset{\triangledown}{\mathbf{S}} + \frac{\lambda_3}{2}\left(\mathbf{D}\mathbf{S} + \mathbf{S}\mathbf{D}\right) + \frac{\lambda_5}{2}\left(\operatorname{Tr}\mathbf{S}\right)\mathbf{D} + \frac{\lambda_6}{2}\left(\mathbf{S} \cdot \mathbf{D}\right)\mathbf{I} = -\mu\left(\mathbf{D} + \lambda_2 \overset{\triangledown}{\mathbf{D}} + \lambda_4 \mathbf{D}^2 + \frac{\lambda_7}{2}\left(\mathbf{D} \cdot \mathbf{D}\right)\mathbf{I}\right)$$

$$\overset{\triangledown}{\mathbf{b}} =_{\mathrm{def}} \frac{\mathrm{d}\mathbf{b}}{\mathrm{d}t} - \left[\nabla \mathbf{v}\right]\mathbf{b} - \mathbf{b}\left[\nabla \mathbf{v}\right]^{\top}$$

Thermodynamics

Is it possible to develop a thermodynamical framework for these models?

Yes, but the classical Coleman–Noll procedure is not very useful.

Bernard D. Coleman. Thermodynamics of materials with memory. *Arch. Ration. Mech. Anal.*, 17:1–46, 1964

Bernard D. Coleman and Walter Noll. The thermodynamics of elastic materials with heat conduction and viscosity. *Arch. Ration. Mech. Anal.*, 13:167–178, 1963

It is better to use the framework based on the maximization of the rate of entropy production.

Hans Ziegler. Some extremum principles in irreversible thermodynamics with application to continuum mechanics. In *Progress in Solid Mechanics, Vol. IV*, pages 91–193. North-Holland, Amsterdam, 1963

K. R. Rajagopal and A. R. Srinivasa. On thermomechanical restrictions of continua. *Proc. R. Soc. Lond., Ser. A, Math. Phys. Eng. Sci.*, 460(2042):631–651, 2004

Entropy

Balance equation for entropy:

$$\rho \frac{\mathrm{d}\eta}{\mathrm{d}t} = \mathrm{div}\left(\frac{\mathbf{q}}{\theta}\right) + \frac{\zeta}{\theta}$$
$$\zeta = \mathbf{T} \cdot \mathbf{D} - \mathbf{q} \cdot \nabla\theta$$

Second law of thermodynamics:

$$\zeta \geq 0$$

Coleman–Noll

Guess:

$$\mathbf{T} =_{\mathrm{def}} \mathfrak{f}(\mathbf{D})$$

Show that:

$$\mathbf{T} \cdot \mathbf{D} = \mathfrak{f}(\mathbf{D}) \cdot \mathbf{D} \geq 0$$

Maximization of the rate of entropy production

Guess:

$$\zeta =_{\rm def} \hat{\zeta}(\mathbf{T}, \mathbf{D}) \geq 0$$

- Find $\mathbf{T}$ such that $\mathbf{T}$ maximizes ζ subject to $\zeta - \mathbf{T} \cdot \mathbf{D} = 0$ as a constraint.
- If necessary, apply other constraints as well. (For example incompressibility $\operatorname{Tr} \mathbf{D} = 0$.)
- The condition for maximum is the constitutive relation, $\mathbf{T} = \mathbf{T}(\mathbf{D})$.

Role of $\mathbf{T}$ and $\mathbf{D}$ can be changed.

Thermodynamically consistent model

Choose a constitutive relation the for rate of dissipation:

$$\zeta = f\left(\operatorname{Tr}\mathbf{D}, \operatorname{Tr}\mathbf{T}, \operatorname{Tr}\mathbf{D}^2, \operatorname{Tr}\mathbf{T}^2, \operatorname{Tr}\mathbf{T}^3, \operatorname{Tr}\mathbf{D}^3, \right.$$
$$\left. \operatorname{Tr}\mathbf{TD}, \operatorname{Tr}\mathbf{T}^2\mathbf{D}, \operatorname{Tr}\mathbf{TD}^2, \operatorname{Tr}\mathbf{T}^2\mathbf{D}^2\right) \geq 0$$

One can think about

$$\zeta = (\operatorname{Tr}\mathbf{T})^2 + \operatorname{Tr}\mathbf{D}^2 + \operatorname{Tr}\mathbf{T}^2 + \left(\operatorname{Tr}\mathbf{T}^3\right)^2 + \left(\operatorname{Tr}\mathbf{D}^3\right)^2 + (\operatorname{Tr}(\mathbf{TD}))^2$$
$$+ \left(\operatorname{Tr}\left(\mathbf{T}^2\mathbf{D}\right)\right)^2 + \left(\operatorname{Tr}\left(\mathbf{TD}^2\right)\right)^2 + \operatorname{Tr}\left(\mathbf{T}^2\mathbf{D}^2\right)$$

Thermodynamically consistent model

Guess:

$$\zeta = 2\mu \mathbf{D} \cdot \mathbf{D} + 2\alpha \frac{\left(\mathbf{T} \cdot \mathbf{D}^2\right)^2}{\mathbf{D} \cdot \mathbf{D}} \geq 0$$

Result:

$$\mathbf{T}_\delta = 2\mu \left(1 - \frac{\alpha}{\mu} \frac{\left(\mathbf{T} \cdot \mathbf{D}^2\right)^2}{\left(\mathbf{D} \cdot \mathbf{D}\right)^2}\right) \mathbf{D} + 2\alpha \frac{\mathbf{T} \cdot \mathbf{D}^2}{\mathbf{D} \cdot \mathbf{D}} \left(\mathbf{TD} + \mathbf{DT} - \frac{2}{3} \left(\mathbf{T} \cdot \mathbf{D}\right) \mathbf{I}\right)$$

Summary

Implicit constitutive relations

Relations of type

$$\mathfrak{f}\left(\mathbf{T},\mathbf{D}\right)=\mathbf{0}$$

or

$$\mathfrak{H}_{s=0}^{+\infty}\left(\mathbf{T}(t-s),\mathbf{C}_t\left(t-s\right)\right)=\mathbf{0}$$

allow one to bring under one unifying theme a much richer and wider class of material response.

Why

Old models are seen form different perspective and new thermodynamically consistent models can be easy developed.

Problems

Physical laws:

$$\rho \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \operatorname{div} \mathbf{T} + \rho \mathbf{b}$$
$$\operatorname{div} \mathbf{v} = 0$$
$$\mathbf{T} = \mathbf{T}^\top$$

Material properties:

$$\mathfrak{f}\left(\mathbf{T}, \mathbf{D}\right) = \mathbf{0}$$

or

$$\mathfrak{H}_{s=0}^{+\infty}\left(\mathbf{T}(t-s), \mathbf{C}_t\left(t-s\right)\right) = \mathbf{0}$$

Mathematical problems: existence and uniqueness of the solution, qualitative properties of the solution, stability, numerical methods