Perspectives on using implicit type constitutive relations in the modelling of the behaviour of non-Newtonian fluids

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Constitutive relations

Governing equations (incompressible homogeneous material):

$$\begin{aligned}
\operatorname{div} \boldsymbol{v} &= 0 \\
\rho \frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} &= \operatorname{div} \mathbb{T} + \rho \boldsymbol{b} \\
\mathbb{T} &= \mathbb{T}^{\top}
\end{aligned}$$

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Constitutive relations (Navier–Stokes), $\mathbb{D} =_{\mathrm{def}} \frac{1}{2}\left(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^\top\right)$:

$$
\mathbb{T} = -p\mathbb{I} + 2\mu\mathbb{D}
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Different perspective, $\operatorname{Tr} \mathbb{D} = \operatorname{div} \boldsymbol{v} = 0$, $\mathbb{T}_\delta =_{\mathrm{def}} \mathbb{T} - \frac{1}{3}\operatorname{Tr}(\mathbb{T})\,\mathbb{I}$:

$$\mathbb{T}_\delta = 2\mu\mathbb{D}$$

Constitutive relations for non-Newtonian fluids

Standard approach: Stress is an function of kinematical variables.

$$\mathbb{T}_\delta = \mathfrak{f}(\mathbb{D})$$

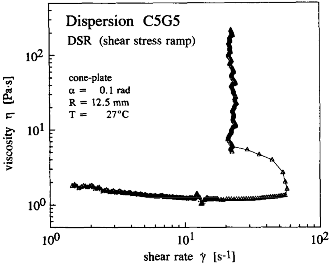
Example:

$$\mathbb{T}_\delta = 2\left(\mu_\infty + \frac{\mu_0 - \mu_\infty}{\left(1 + \alpha \left|\mathbb{D}\right|^2\right)^{\frac{n}{2}}}\right)\mathbb{D}$$

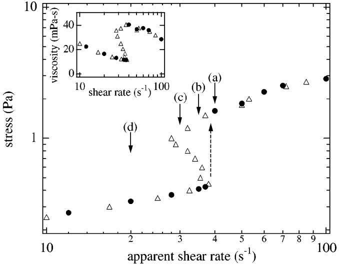
Pierre J. Carreau. Rheological equations from molecular network theories. *J. Rheol.*, 16(1):99–127, 1972

This approach dominates the standard phenomenological theory of constitutive relations.

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



(a) Polymer dispersion C5G5 (styren/ethyl acrylate copolymer particles in glycol), shear stress ramp experiment.



(b) Steady-state stress/shear–rate behaviour; constant applied shear stress (triangles) and constant applied shear rate (circles), TTAA/NaSal solution.

Figure: Experimental data for some fluids.

H. M. Laun. Normal stresses in extremely shear thickening polymer dispersions. *J. Non-Newton. Fluid Mech.*, 54:87–108, 1994

Philippe Boltenhagen, Yuntao Hu, E. F. Matthys, and D. J. Pine. Observation of bulk phase separation and coexistence in a sheared micellar solution. *Phys. Rev. Lett.*, 79:2359–2362, Sep 1997

Constitutive relations for non-Newtonian fluids

Alternative approach: There is a relation between stress and kinematical variables.

$$\mathfrak{f}(\mathbb{T}_\delta, \mathbb{D}) = \mathbb{0}$$

Example:

$$\mathbb{T}_\delta = 2\left(\mu_\infty + (\mu_0 - \mu_\infty)\,\mathrm{e}^{-\frac{|\mathbb{T}_\delta|}{\tau_0}}\right)\mathbb{D}$$

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

Constitutive relations for non-Newtonian fluids

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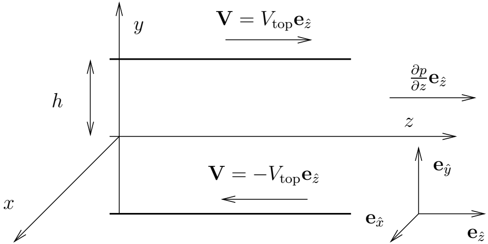
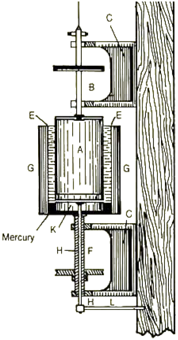
Shear stress and shear rate



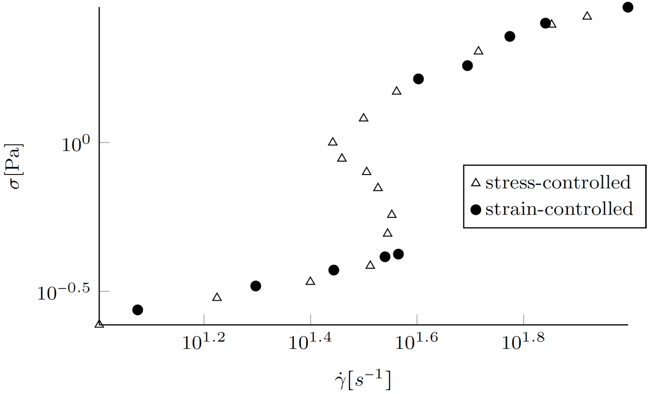


$$\mathbb{T} = \begin{bmatrix} \mathrm{T}_{\hat{x}\hat{x}} & 0 & 0 \\ 0 & \mathrm{T}_{\hat{y}\hat{y}} & \mathrm{T}_{\hat{y}\hat{z}} \\ 0 & \mathrm{T}_{\hat{z}\hat{y}} & \mathrm{T}_{\hat{z}\hat{z}} \end{bmatrix} \qquad \mathbb{D} = \frac{1}{2}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\mathrm{d}v^{\hat{z}}}{\mathrm{d}y} \\ 0 & \frac{\mathrm{d}v^{\hat{z}}}{\mathrm{d}y} & 0 \end{bmatrix}$$

$$\sigma =_{\text{def}} \mathrm{T}_{\hat{y}\hat{z}} \quad \text{(shear stress)} \qquad \dot{\gamma} =_{\text{def}} \frac{\mathrm{d}v^{\hat{z}}}{\mathrm{d}y} \quad \text{(shear rate)}$$

Example

$\mathbb{T} \approx \sigma$ (shear stress) $\mathbb{D} \approx \dot{\gamma}$ (shear rate, strain rate)



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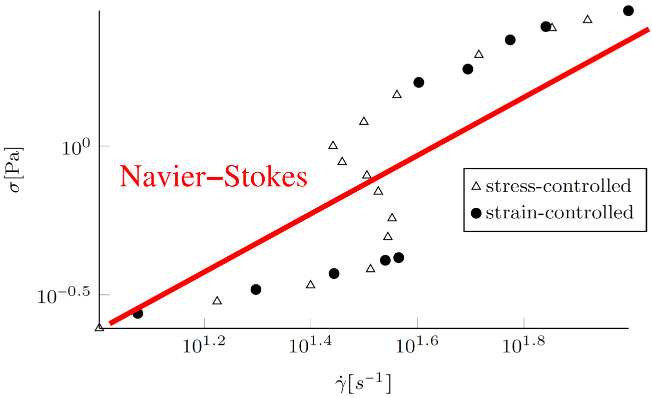

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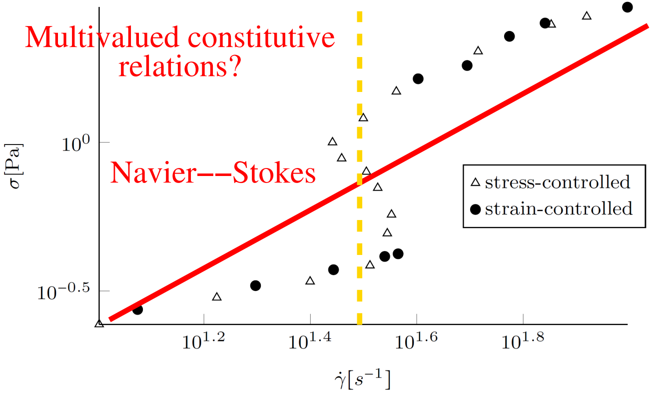

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One-dimensional implicit type relations

One dimensional data:

$$\mathbb{T} \approx \sigma \text{ (shear stress)} \qquad \mathbb{D} \approx \dot{\gamma} \text{ (shear rate, strain rate)}$$

Standard approach (does not work):

$$\mathbb{T}_\delta = \mathfrak{f}(\mathbb{D})$$

Alternative approach:

$$\mathfrak{f}(\mathbb{T}_\delta, \mathbb{D}) = \mathbb{0} \qquad \text{or} \qquad \mathbb{D} = \mathfrak{f}(\mathbb{T}_\delta)$$

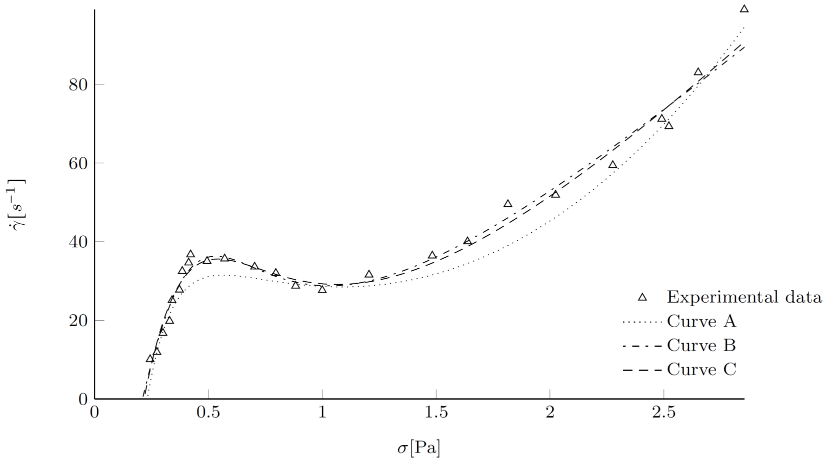
Curves:

$$\dot{\gamma} = \mathrm{e}^{-a\sigma}\left(a_1\sigma + b_1\right) + \left(1 - \mathrm{e}^{-b\sigma}\right)\left(a_2\sigma + b_2\right) \tag{A}$$

$$\dot{\gamma} = \frac{p_1\sigma^3 + p_2\sigma^2 + p_3\sigma + p_4}{\sigma^2 + q_1\sigma + q_2} \tag{B}$$

$$\dot{\gamma} = \left(\alpha\left(1 + \beta\sigma^2\right)^n + \gamma\right)\sigma \tag{C}$$

One dimensional implict type relations – curve fitting



Reconstruction of the tensorial constitutive relation from one-dimensional data

Task:

$$f(\sigma, \dot{\gamma}) = 0 \mapsto \mathfrak{f}(\mathbb{T}_\delta, \mathbb{D}) = \mathbb{0}$$

Experimental data:

$$\mathbb{T} = \begin{bmatrix} \mathrm{T}_{\hat{x}\hat{x}} & 0 & 0 \\ 0 & \mathrm{T}_{\hat{y}\hat{y}} & \mathrm{T}_{\hat{y}\hat{z}} \\ 0 & \mathrm{T}_{\hat{z}\hat{y}} & \mathrm{T}_{\hat{z}\hat{z}} \end{bmatrix} \qquad \mathbb{D} = \frac{1}{2} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\mathrm{d}v^{\hat{z}}}{\mathrm{d}y} \\ 0 & \frac{\mathrm{d}v^{\hat{z}}}{\mathrm{d}y} & 0 \end{bmatrix}$$

$$\sigma =_{\mathrm{def}} \mathrm{T}_{\hat{y}\hat{z}} \quad \text{(shear stress)} \qquad \dot{\gamma} =_{\mathrm{def}} \frac{\mathrm{d}v^{\hat{z}}}{\mathrm{d}y} \quad \text{(shear rate)}$$

Reconstruction of the tensorial constitutive relation from one-dimensional data – curve B

Task:

$$f(\sigma, \dot{\gamma}) = 0 \mapsto \mathfrak{f}(\mathbb{T}_\delta, \mathbb{D}) = \mathbb{0}$$

Fit of one dimensional experimental data:

$$\left(\sigma^2 + q_1\sigma + q_2\right)\dot{\gamma} = \left(p_1\sigma^2 + p_2\sigma + p_3\right)\sigma$$

Alternatives:

$$\left(\left|\mathbb{T}_\delta\right|^2 + q_1\left|\mathbb{T}_\delta\right| + q_2\right)\mathbb{D} = \left(p_1\left|\mathbb{T}_\delta\right|^2 + p_2\left|\mathbb{T}_\delta\right| + p_3\right)\mathbb{T}_\delta$$

$$\left(\mathbb{T}_\delta^2\mathbb{D} + \mathbb{D}\mathbb{T}_\delta^2\right)_\delta + \tilde{q}_1\left(\mathbb{T}_\delta\mathbb{D} + \mathbb{D}\mathbb{T}_\delta\right)_\delta + q_2\mathbb{D} = \left(p_4\left|\mathbb{T}_\delta\right|^2 + p_3\left|\mathbb{T}_\delta\right| + p_2\right)\mathbb{T}_\delta$$

$$\left(\mathbb{T}_\delta^2\mathbb{D} + \mathbb{D}\mathbb{T}_\delta^2\right)_\delta + q_1\left|\mathbb{T}_\delta\right|\mathbb{D} + q_2\mathbb{D} = \left(p_4\left|\mathbb{T}_\delta\right|^2 + p_2\right)\mathbb{T}_\delta + p_3\left(\mathbb{T}_\delta^2\right)_\delta$$

Non-newtonian fluids and normal stress differences

(a) Weissenberg effect.

(b) Barus effect.

Normal stress differences:

$$N_1 =_{\mathrm{def}} \mathrm{T}_{\hat{z}\hat{z}} - \mathrm{T}_{\hat{y}\hat{y}}$$
$$N_2 =_{\mathrm{def}} \mathrm{T}_{\hat{y}\hat{y}} - \mathrm{T}_{\hat{x}\hat{x}}$$

Non-newtonian fluids and normal stress differences

Navier–Stokes, $\mathbb{T} = -p\mathbb{I} + 2\mu\mathbb{D}$:

$$\begin{bmatrix} \mathrm{T}_{\hat{x}\hat{x}} & 0 & 0 \\ 0 & \mathrm{T}_{\hat{y}\hat{y}} & \mathrm{T}_{\hat{y}\hat{z}} \\ 0 & \mathrm{T}_{\hat{z}\hat{y}} & \mathrm{T}_{\hat{z}\hat{z}} \end{bmatrix} = -p \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \mu \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\mathrm{d}v^{\hat{z}}}{\mathrm{d}y} \\ 0 & \frac{\mathrm{d}v^{\hat{z}}}{\mathrm{d}y} & 0 \end{bmatrix}$$

A non-newtonian model, $\mathbb{T} = -p\mathbb{I} + 2\mu\mathbb{D} + 4\tilde{\mu}\mathbb{D}^2$:

$$\begin{bmatrix} \mathrm{T}_{\hat{x}\hat{x}} & 0 & 0 \\ 0 & \mathrm{T}_{\hat{y}\hat{y}} & \mathrm{T}_{\hat{y}\hat{z}} \\ 0 & \mathrm{T}_{\hat{z}\hat{y}} & \mathrm{T}_{\hat{z}\hat{z}} \end{bmatrix} = -p \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \mu \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\mathrm{d}v^{\hat{z}}}{\mathrm{d}y} \\ 0 & \frac{\mathrm{d}v^{\hat{z}}}{\mathrm{d}y} & 0 \end{bmatrix} + \tilde{\mu} \begin{bmatrix} 0 & 0 & 0 \\ 0 & \left(\frac{\mathrm{d}v^{\hat{z}}}{\mathrm{d}y}\right)^2 & 0 \\ 0 & 0 & \left(\frac{\mathrm{d}v^{\hat{z}}}{\mathrm{d}y}\right)^2 \end{bmatrix}$$

Key question

How to develop reasonable constitutive relations?

General algebraic implicit constitutive relation – restrictions

Incompressible, homogeneous, isotropic fluid:

$$\alpha_1 \mathbb{T}_\delta + \alpha_2 \mathbb{D} + \alpha_3 \left(\mathbb{T}_\delta^2\right)_\delta + \alpha_4 \left(\mathbb{D}^2\right)_\delta + \alpha_5 \left(\mathbb{T}_\delta \mathbb{D} + \mathbb{D}\mathbb{T}_\delta\right)_\delta + \alpha_6 \left(\mathbb{T}_\delta^2 \mathbb{D} + \mathbb{D}\mathbb{T}_\delta^2\right)_\delta + \alpha_7 \left(\mathbb{T}_\delta \mathbb{D}^2 + \mathbb{D}^2 \mathbb{T}_\delta\right)_\delta + \alpha_8 \left(\mathbb{T}_\delta^2 \mathbb{D}^2 + \mathbb{D}^2 \mathbb{T}_\delta^2\right)_\delta = \mathbb{0}$$

Second law of thermodynamics:

$$\mathbb{T} : \mathbb{D} \geq 0$$

Dynamical admissibility in simple shear flow:

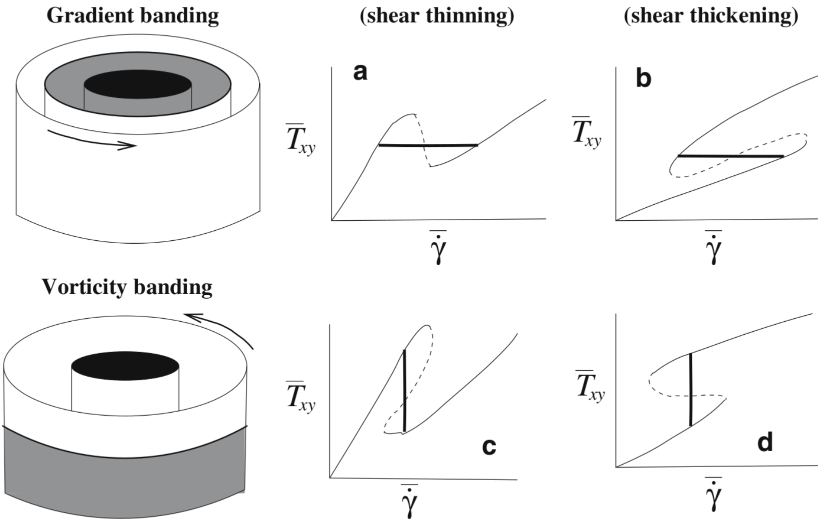
$$\boldsymbol{v} = \frac{V_{\mathrm{top}}}{h} \boldsymbol{e}_{\hat{z}}$$

T. Perlácová and V. Průša. Tensorial implicit constitutive relations in mechanics of incompressible non-Newtonian fluids. *J. Non-Newton. Fluid Mech.*, 216:13–21, 2015

Summary

- Some experimental data that can not be interpreted using the standard models $\mathbb{T}_\delta = \mathfrak{f}(\mathbb{D})$.
- Implicit constitutive relations $\mathfrak{f}(\mathbb{T}_\delta, \mathbb{D}) = 0$ provide a tool how to develop constitutive models.
- Building a model using one-dimensional data is always a problem. (Rethinking of experimental procedures is necessary.)
- Construction of a three dimensional fully implicit tensorial constitutive relations (thermodynamic background).

Nonmonotone response – gradient and vorticity banding



Peter D. Olmsted. Perspectives on shear banding in complex fluids. *Rheol. Acta*, 47(3):283–300, 2008

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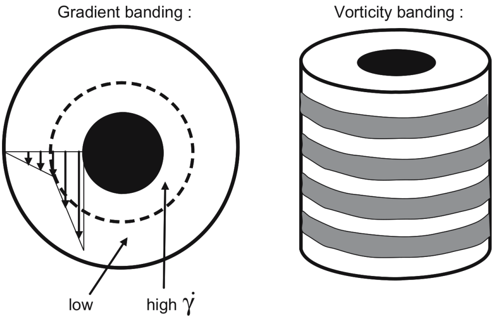

Jan K. G. Dhont and Wim J. Briels. Gradient and vorticity banding. *Rheol. Acta*, 47(3):257–281, 2008

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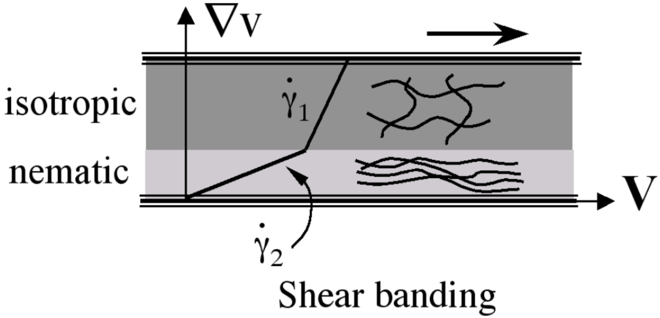

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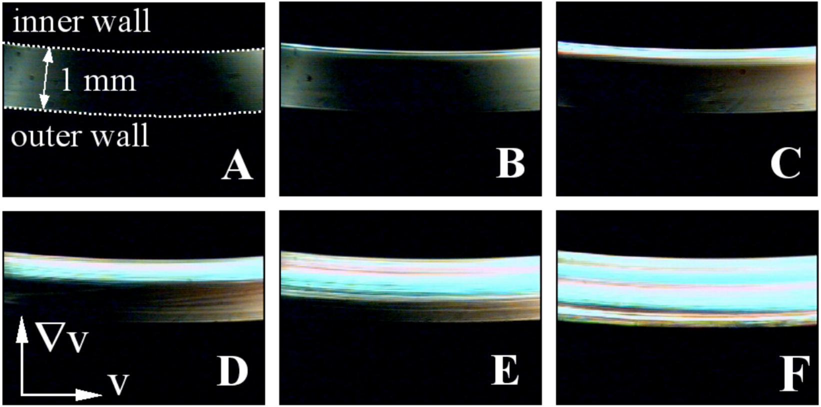

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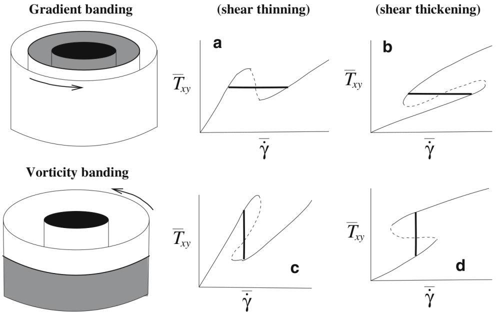

Design goals:

- Non-monotone response in simple shear flow.
- Viscoelasticity. (Time dependent flows.)
- Normal stress differences. (Three dimensional effects.)

Conclusion

- New mathematical models are needed.
- Implicit constitutive relations are of interest.
- Non-monotone response leads to interesting dynamics.

$$
\begin{aligned}
\operatorname{div} \boldsymbol{v} &= 0 \\
\rho \frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} &= \operatorname{div} \mathbb{T} + \rho \boldsymbol{b} \\
\mathbb{T} &= \mathbb{T}^\top \\
\mathfrak{g}(\mathbb{T}_\delta, \mathbb{D}) &= \mathbb{0}
\end{aligned}
$$