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):

\[ \text{div } \mathbf{v} = 0 \]

\[ \rho \frac{d\mathbf{v}}{dt} = \text{div } \mathbb{T} + \rho \mathbf{b} \]

\[ \mathbb{T} = \mathbb{T}^T \]
Constitutive relations

Governing equations (incompressible homogeneous material):

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\[ \mathbf{T} = \mathbf{T}^\top \]

Constitutive relations (Navier–Stokes), \( \mathbb{D} = \text{def} \frac{1}{2} (\nabla \mathbf{v} + \nabla \mathbf{v}^\top) \):

\[ \mathbf{T} = -p\mathbb{I} + 2\mu \mathbb{D} \]
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Constitutive relations (Navier–Stokes), \( \mathcal{D} = \text{def} \, \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^\top) : \)

\[ \mathbf{T} = -p \mathbf{1} + 2\mu \mathcal{D} \]

Different perspective, \( \text{Tr } \mathcal{D} = \text{div } \mathbf{v} = 0, \mathbf{T}_\delta = \text{def } \mathbf{T} - \frac{1}{3} \text{Tr } (\mathbf{T}) \mathbf{1} : \)

\[ \mathbf{T}_\delta = 2\mu \mathcal{D} \]
Constitutive relations for non-Newtonian fluids

Standard approach: Stress is an function of kinematical variables.

\[ \mathbb{T}_\delta = f(\mathbb{D}) \]

Example:

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


This approach dominates the standard phenomenological theory of constitutive relations.

(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.


Constitutive relations for non-Newtonian fluids

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

\[ f(T_{\delta}, \mathcal{D}) = 0 \]

Example:

\[ T_{\delta} = 2 \left( \mu_{\infty} + (\mu_0 - \mu_{\infty}) e^{-\frac{|T_{\delta}|}{\tau_0}} \right) \mathcal{D} \]

Constitutive relations for non-Newtonian fluids

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

\[ f(T_\delta, D) = 0 \]
Shear stress and shear rate

\[ \mathbf{V} = V_{\text{top}} \hat{e}_z \]

\[ \mathbf{V} = -V_{\text{top}} \hat{e}_z \]

\[ T = \begin{bmatrix} T_{\hat{x}\hat{x}} & 0 & 0 \\ 0 & T_{\hat{y}\hat{y}} & T_{\hat{y}\hat{z}} \\ 0 & T_{\hat{z}\hat{y}} & T_{\hat{z}\hat{z}} \end{bmatrix} \]

\[ \mathbf{D} = \frac{1}{2} \begin{bmatrix} 0 & 0 & 0 & \frac{d\mathbf{v}^2}{dy} \\ 0 & 0 & \frac{d\mathbf{v}^2}{dy} & 0 \end{bmatrix} \]

\[ \sigma = \text{def } T_{\hat{y}\hat{z}} \quad \text{(shear stress)} \]

\[ \dot{\gamma} = \text{def } \frac{d\mathbf{v}^2}{dy} \quad \text{(shear rate)} \]
\[ T \approx \sigma \text{ (shear stress)} \quad D \approx \dot{\gamma} \text{ (shear rate, strain rate)} \]

Example

\[ \mathbf{T} \approx \sigma \text{ (shear stress) } \quad \mathbf{D} \approx \dot{\gamma} \text{ (shear rate, strain rate)} \]

Navier–Stokes

Example

\[ T \approx \sigma \text{ (shear stress) } \quad \mathbb{D} \approx \dot{\gamma} \text{ (shear rate, strain rate)} \]

Multivalued constitutive relations?

Navier--Stokes

One-dimensional implicit type relations

One dimensional data:

\[ T \approx \sigma \text{ (shear stress)} \quad D \approx \dot{\gamma} \text{ (shear rate, strain rate)} \]

Standard approach (does not work):

\[ T_\delta = f(D) \]

Alternative approach:

\[ f(T_\delta, D) = 0 \quad \text{or} \quad D = f(T_\delta) \]

Curves:

\[ \dot{\gamma} = e^{-a\sigma} (a_1 \sigma + b_1) + \left(1 - e^{-b\sigma}\right) (a_2 \sigma + b_2) \quad (A) \]

\[ \dot{\gamma} = \frac{p_1 \sigma^3 + p_2 \sigma^2 + p_3 \sigma + p_4}{\sigma^2 + q_1 \sigma + q_2} \quad (B) \]

\[ \dot{\gamma} = \left(\alpha \left(1 + \beta \sigma^2\right)^n + \gamma\right) \sigma \quad (C) \]
One dimensional implicit type relations – curve fitting
Reconstruction of the tensorial constitutive relation from one-dimensional data

Task:

\[ f(\sigma, \dot{\gamma}) = 0 \implies f(T_\delta, D) = 0 \]

Experimental data:

\[ T = \begin{bmatrix} T_{\hat{x}\hat{x}} & 0 & 0 \\ 0 & T_{\hat{y}\hat{y}} & T_{\hat{y}\hat{z}} \\ 0 & T_{\hat{z}\hat{y}} & T_{\hat{z}\hat{z}} \end{bmatrix} \quad D = \frac{1}{2} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{d\nu^2}{dy} \\ 0 & \frac{d\nu^2}{dy} & 0 \end{bmatrix} \]

\[ \sigma = \text{def } T_{\hat{y}\hat{z}} \quad \text{(shear stress)} \quad \dot{\gamma} = \text{def } \frac{d\nu^2}{dy} \quad \text{(shear rate)} \]
Reconstruction of the tensorial constitutive relation from one-dimensional data – curve B

Task:

\[ f(\sigma, \dot{\gamma}) = 0 \mapsto f(T_\delta, D) = 0 \]

Fit of one dimensional experimental data:

\[ (\sigma^2 + q_1 \sigma + q_2) \dot{\gamma} = (p_1 \sigma^2 + p_2 \sigma + p_3) \sigma \]

Alternatives:

\[ \left( |T_\delta|^2 + q_1 |T_\delta| + q_2 \right) D = \left( p_1 |T_\delta|^2 + p_2 |T_\delta| + p_3 \right) T_\delta \]

\[ (T^2_\delta D + DT^2_\delta)_\delta + \tilde{q}_1 (T_\delta D + DT_\delta)_\delta + q_2 D = \left( p_4 |T_\delta|^2 + p_3 |T_\delta| + p_2 \right) T_\delta \]

\[ (T^2_\delta D + DT^2_\delta)_\delta + q_1 |T_\delta| D + q_2 D = \left( p_4 |T_\delta|^2 + p_2 \right) T_\delta + p_3 (T^2_\delta)_\delta \]
Non-newtonian fluids and normal stress differences

(a) Weissenberg effect.  
(b) Barus effect.

Normal stress differences:

\[ N_1 = \text{def } T_{zz} - T_{yy} \]
\[ N_2 = \text{def } T_{yy} - T_{xx} \]
Non-newtonian fluids and normal stress differences

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

\[
\begin{bmatrix}
T_{\hat{x}\hat{x}} & 0 & 0 \\
0 & T_{\hat{y}\hat{y}} & T_{\hat{y}\hat{z}} \\
0 & T_{\hat{z}\hat{y}} & T_{\hat{z}\hat{z}}
\end{bmatrix} = -p \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \mu \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{dv^2}{dy} \\ 0 & \frac{dv^2}{dy} & 0 \end{bmatrix}
\]

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

\[
\begin{bmatrix}
T_{\hat{x}\hat{x}} & 0 & 0 \\
0 & T_{\hat{y}\hat{y}} & T_{\hat{y}\hat{z}} \\
0 & T_{\hat{z}\hat{y}} & T_{\hat{z}\hat{z}}
\end{bmatrix} = -p \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \mu \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{dv^2}{dy} \\ 0 & \frac{dv^2}{dy} & 0 \end{bmatrix} + \tilde{\mu} \begin{bmatrix} 0 & 0 & 0 \\ 0 & \left( \frac{dv^2}{dy} \right)^2 & 0 \\ 0 & 0 & \left( \frac{dv^2}{dy} \right)^2 \end{bmatrix}
\]
Key question

How to develop reasonable constitutive relations?
General algebraic implicit constitutive relation – restrictions

Incompressible, homogeneous, isotropic fluid:

\[
\alpha_1 T_\delta + \alpha_2 D + \alpha_3 (T^2_\delta)_\delta + \alpha_4 (D^2)_\delta + \alpha_5 (T_\delta D + DT_\delta)_\delta + \alpha_6 (T^2_\delta D + DT^2_\delta)_\delta \\
+ \alpha_7 (T_\delta D^2 + D^2 T_\delta)_\delta + \alpha_8 (T^2_\delta D^2 + D^2 T^2_\delta)_\delta = 0
\]

Second law of thermodynamics:

\[ T : D \geq 0 \]

Dynamical admissibility in simple shear flow:

\[ \mathbf{v} = \frac{V_{\text{top}}}{h} \mathbf{e}_z \]

Some experimental data that can not be interpreted using the standard models $\mathbb{T}_\delta = f(\mathbb{D})$.

Implicit constitutive relations $f(\mathbb{T}_\delta, \mathbb{D}) = 0$ 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

Gradient banding

Vorticity banding

Nonmonotone response – gradient and vorticity banding

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Nonmonotone response – gradient and vorticity banding

Key question

How to develop reasonable constitutive relations?

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.

\[
\begin{align*}
\text{div } \mathbf{v} &= 0 \\
\rho \frac{\text{d} \mathbf{v}}{\text{d} t} &= \text{div } \mathbf{T} + \rho \mathbf{b} \\
\mathbf{T} &= \mathbf{T}^\top \\
g(\mathbf{T}_\delta, \mathbf{D}) &= 0
\end{align*}
\]