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The Solution for Constitutive Modelling of Polymer Melts?

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Introduction
The difficulty in constitutive modelling of polymer melts is to get a correct non-linear behaviour in both elongation and shear. The recently proposed Pom-Pom model [1], is a major step forward in solving this problem. In this work, an extension is proposed to improve the performance of the Pom-Pom model. Eventually, the objective is to calculate visco-elastic polymer melt flows in characteristic geometries under processing conditions.

The Pom-Pom model
The model is based on the schematic configuration of figure 1.

Fig. 1: Schematic Pom-Pom ‘molecule’.

Original differential decoupled equations [1, 2]:
\[ \nabla A + \frac{1}{\lambda} [ A - \frac{1}{\lambda} I ] = 0, \quad S = \frac{\Lambda}{\lambda} \]
\[ \Rightarrow \dot{S} + [ D : S ] S + \frac{1}{\lambda_{\alpha}} [ 3 \alpha \Lambda S : S \\
+ (1 - \alpha - 3 \alpha \Lambda I_{s,s}) S - \frac{(1 - \alpha)}{3} I ] = 0 \]

\[ \dot{S} = \Lambda [ D : S ] - \frac{1}{\lambda} (\Lambda - 1) \forall \Lambda \leq q \]

\[ \tau = G_0 \left( 3 \Lambda^2 S - I \right) \]

with \( \lambda = \lambda_{\alpha} e^{-\nu(\Lambda-1)} \), \( \nu = \frac{2}{7} \).

Limitations of original differential Pom-Pom model:
- Unbounded orientation for \( \dot{\varepsilon}_{\alpha 0} > 1 \).
- Non-smooth elongational viscosity due to maximum stretch condition.
- \( \Psi_2 = 0 \).

The eXtended Pom-Pom (XPP) model resolves these limitations, by eliminating the maximum stretch condition, and modifying the orientation and stretch:
\[ \dot{S} + [ D : S ] S + \frac{1}{\lambda_{\alpha}} \left[ 3 \alpha \Lambda S : S \\
+ (1 - \alpha - 3 \alpha \Lambda I_{s,s}) S - \frac{(1 - \alpha)}{3} I \right] = 0, \]
\[ \dot{\Lambda} = \Lambda [ D : S ] - \frac{1}{\lambda} (\Lambda - 1) \]

The XPP model can be written as a single equation:
\[ \dot{\tau} + \lambda (\tau)^{-1} \cdot \tau = 2 G_0 D \]

with \( \lambda (\tau)^{-1} = \frac{1}{\lambda_{\alpha}} \left[ \frac{\alpha}{\alpha - 1} \tau + f(\tau)^{-1} I + G_0 (f(\tau)^{-1} - 1) \right] \),
\[ \frac{1}{\lambda_{\alpha}} f(\tau)^{-1} = \frac{1}{\lambda_{\alpha}} (1 - \frac{1}{\alpha}) + \frac{1}{\lambda_{\alpha}} \left( \frac{\alpha f}{3 \alpha^2} - \frac{\alpha f}{3 \alpha^2} \right) \]

and \( \Lambda = \sqrt{1 + \frac{1}{\lambda_{\alpha}} \cdot \frac{\alpha f}{3 \alpha^2}} \).

The Performance
A 4 modes XPP model is used for predicting data of an LDPE (DSM, Stamylan LD 2008 XC43) melt.

Uniaxial Elongation
The non-linear parameters, \( q \) and \( \frac{\lambda_{\alpha}}{\lambda_{\alpha}} \), are fitted on uniaxial elongational data [3] only.

Simple Shear
Without changing the parameters, the correct behaviour for shear data [4] is predicted.

Complex Flow
A complex flow with combined shear/elongation regions, the cross slot flow, is investigated.

Conclusions
- Excellent quantitative agreement in both elongation and shear.
- Smooth results, by eliminating maximum stretch condition.
- Fitting of non-linear parameters \( q \) and \( \frac{\lambda_{\alpha}}{\lambda_{\alpha}} \) on uniaxial experimental data only.
- Good quantitative performance in complex flow.

References:

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