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Abstract
We use a differential constitutive equation to model the flow of a viscoelastic flow in a cross-slot geometry, which is known to exhibit bistability above a critical flow rate. The novelty lies in two asymmetric modifications to the geometry, which causes a change in the bifurcation diagram such that one of the stable solutions becomes disconnected from the solution at low flow speeds. First we show that it is possible to mirror one of the modifications such that the system can be forced to the disconnected solution. Then we show that a slow decrease of the flow rate, can cause the system to go through a drastic change on a short time scale, also known as a catastrophe. The short time scale could lead to a precise and simple experimental measurement of the flow conditions at which the viscoelastic catastrophe occurs. Since the phenomena is intrinsically related to the extensional rheology of the fluid, we propose to exploit the phenomena for in-line extensional rheometry.

Keywords: viscoelastic catastrophe, bistability, cross-slot, FENE-CR, extensional rheology, microfluidic, COMSOL

1. Introduction

Whenever flexible objects or large molecules are dissolved in a fluid, the flow can give rise to stretching and orientation of these constituents, which in turn can lead to stresses that affect the flow such that a feedback is created. This can result in upstream vortices, instabilities or bistability in what is collectively referred to as viscoelastic effects. Experiments with weakly elastic fluids tend to be dominated by inertia, but the relative magnitude of inertial to viscoelastic effects vanishes as the characteristic length scale is reduced, and this scaling law constitutes the foundation for micro-rheometry [1,2]. The properties of viscoelastic fluids in shear flow is important for pipe flow and lubrication, but complex flows involving contractions and/or obstacles tend to emphasize the extensional properties of these fluids. The cross-slot geometry illustrated in figure 1 give rise to an extensional flow near the stagnation point in the center. Therefore it has been suggested as an extensional micro-rheometer, but often in the context of a birefringence setup [3] and with the tendency for bistability at moderate elasticity viewed as a limiting factor.

Figure 1: The viscoelastic flow in a cross is symmetric in the regime of low elasticity (a), but the symmetric flow becomes unstable in the regime of moderate elasticity. Instead two asymmetric solutions appear, (b) and (c).

The paper is based on simulation of differential constitutive models, and with these tools we predict that it is possible to generate a catastrophe due to viscoelastic effects, that is, an abrupt change in the flow pattern un-
under slow and smooth variations in the input parameters. The abrupt nature of the catastrophe ought to permit detection by simple means, e.g. polarized light or ultrasonic response, and the conditions at which the catastrophe occurs depends on the extensional rheology of the fluid. Therefore we suggest to use it as an extensional micro-rheometer, as the reproducibility is potentially only limited by the continuity of the fluid and the quality of the pumps. The non-ideal extensional flow is a disadvantage, but many applications are far from ideal and in some cases more weight might be put on the simplicity of construction and/or the in-line monitoring capability provided by the confined nature of the device.

The article is structured in four parts: First the modeling of a viscoelastic FENE-CR fluid is described. Then the features of the symmetric cross-slot geometry are sketched, before the changes needed to generate the catastrophe are described on an abstract level. Finally the high-level finite element package. The W eissenberg number, 

\[ \beta = \frac{\eta_s}{\eta_s + \eta_p}, \]

where \( \nu_{\text{char}} \) is a characteristic velocity. \( \beta \) is the solvent to total viscosity ratio, and it expresses the proportion of viscous effects due to the solvent. \( \beta = 1 \) thus corresponds to a Newtonian fluid, while \( \beta = 0 \) and \( a_{\text{max}} \rightarrow \infty \) results in particularly strong elastic effects in what is usually referred to as the Upper Convected Maxwell model. The Weissenberg number, \( \text{We} \), expresses the strength of elastic to viscous effects for the dumbbells.

We solve the set of equations \((2-6)\) using an implementation in COMSOL Multiphysics, a commercial high-level finite element package.

3. The Symmetric Cross-Slot

For \( Q_1 = Q_2 \) and \( L_{\text{out,up}} = L_{\text{out,down}} \), figure 2 illustrate the symmetric cross. We will not show new simulations for this as numerous results already exists \([8, 9, 10, 11]\), but just describe the qualitative features of the symmetric case.

We define the Weissenberg number using the total flow rate \( Q_1 + Q_2 \),

\[ \text{We} = \frac{Q_1 + Q_2}{2H^2}. \]  

Figure 3(a) sketches the hydraulic resistance of the symmetric cross-slot as a function of the Weissenberg number. The point of maximum resistance corresponds to
the point of bistability, and characteristic plots of the
trace of the conformation tensor are shown in figure\ref{fig:3}(b)
and (c). Note that a similar plot of the dissipation would
also give a maximum at the point of bistability in the
case of a flow rate driven setup, where as the point of
bistability would be a dissipation minimum in the case
of a pressure driven setup. Regardless of the setup, the
two asymmetric solutions give rise to the same resis-
tance/dissipation for the same Weissenberg number, and
one can think of the rotation of the flow as a way for the
fluid to avoid strong extension in the central stagnation
topic.

(\textbf{a})

(\textbf{b})

(\textbf{c})

Figure 3: (a) is a sketch of the hydraulic in the cross-slot as a func-
tion of the Weissenberg number with the maximum corresponding to
the point of bistability. The red line represents an unstable symmet-
ric solution. (b) and (c) show the trace of the conformation tensor
on a logarithmic scale together with streamlines before and after the
bistability sets in. The stream function is computed and used to plot
streamlines in red.

4. Generating the Catastrophe

We suggest to embrace the bistable character of the
cross-slot geometry by changing the nature of thisphe-
nomenon such that the point of bistability can be used
as a fingerprint of the fluids extensional properties. It
is possible to create an abrupt transient effect – a catas-
trophe – by introducing two asymmetries such that the
double symmetry of the cross-slot is broken, leaving one
of the stable solutions disconnected from the solution at
low flow rates, see figure\ref{fig:4}b).

(a)

(b)

Figure 4: A pitchfork bifurcation is illustrated in (a) with rotation as
solution variable on the y-axis. Red and blue areas represent areas
with increasing clock- and counterclockwise rotation, respectively.
The insets show the symmetric and two asymmetric solutions at their
respective positions in the diagram. Two asymmetric modifications
can give rise to the bifurcation shown in (b), where one of the stable
solutions has become disconnected from the solution at low flow rates.

The asymmetry can be introduced in terms of boundary
conditions, geometry or perhaps even volume
forces, but for our purposes it is imperative that one of
the asymmetries can be flipped, as this enables the de-
vice to be set in the disconnected state as illustrated in
figure\ref{fig:5}. Please take note of the green numbers in fig-
ure\ref{fig:5} since we refer to them throughout the rest of the
text. #1 \xrightarrow{} #2, the system is set in one of the states,
and then one of the asymmetries is flipped [#2 \xrightarrow{} #3],
before the general flow rate (the bifurcation parameter)
is slowly decreased [#3 \xrightarrow{} #6] which gives rise to a
equivalent slow change in the flow until the catastrophe
occurs [#4 \xrightarrow{} #5]. This happens at a particular criti-

cal flow rate, which is characteristic for the extensional
rheology of the working fluid.

5. The Asymmetric Cross-Slot

The asymmetric cross differs from the symmetric one
by having different inlet flow rates as well as outlet
lengths as sketched in figure\ref{fig:6}. We investigate the case of having an upper outlet
length of $9H$, and a lower outlet length equal to half
that. We use the inlet flow rates as control parameters,
and we vary them slowly in time to produce the condi-
tions described in section\ref{sec:4} and illustrated in figure\ref{fig:7}

\begin{equation}
Q_1 = \left(\xi + [1 - \xi] \text{st}^3(\tilde{r})\right)
\end{equation}
the total flow rate as defined in equation (7).

\[ \xi = \frac{\chi}{\chi - 1} \]

\[ Q_2 = \left( \frac{1}{\xi} - 1 \right) s_{\xi 2}^{\#}(t) \]

\[ Q_1 = \left( \frac{\chi}{\chi - 1} + s_{\xi 1}^{\#}(t) \right) \]

where \( \xi \) is the ratio between the inlet flow rates, while \( \chi \) is the ratio of maximum and minimum Weissenberg numbers – due to the fact that these are proportional to the total flow rate as defined in equation (7).

We set the maximum Weissenberg number to 1.14, \( \xi = 0.3, \chi = 2.5, d_{\text{max}} = 100 \) and \( \beta = 0.05 \). \( s_{\xi 1}^{\#}(t), s_{\xi 2}^{\#}(t) \) and \( s_{\xi 0}^{\#}(t) \) are step functions given by

\[ s(t) = \begin{cases} 0 & \text{for } t < t_{\text{start}} \\ 0.5 + 1.5(t - 2)^3 & \text{for } t_{\text{start}} \leq t \leq t_{\text{end}} \\ 1 & \text{for } t \geq t_{\text{end}} \end{cases} \]

\[ \bar{t} = \frac{t - (t_{\text{start}} + t_{\text{end}})/2}{t_{\text{end}} - t_{\text{start}}} \]

\[ T_{\text{step}} = \frac{(t_{\text{end}} - t_{\text{start}})}{\text{We}_{\text{max}}} \]

with \( t_{\text{start}} \) equal to 0, \( T_{\text{step}} \) and \( 2T_{\text{step}} \), respectively. This way we make a single transient simulation that is in fact a collection of quasi-steady solutions to a range of Weissenberg numbers. For the time stepping we use an implicit scheme with adaptive step size, such that slow variation of the Weissenberg number does not increase the total computation time.

We calculate the dissipation (using the Frobenius product denoted with colon)

\[ \phi = \int_\Omega \nabla v : \left( \eta_s [\nabla v + (\nabla v)^T] + \tau \right) d\Omega, \]

where \( \phi \) is the dissipation, \( \eta_s \) is the viscosity, \( \nabla v \) is the velocity gradient, and \( \tau \) is the stress tensor.

The timescale of the jump does not scale with the jump magnitude. The magnitude of the jump is important for a practical realization, but this is completely dependent on the nature of the detection principle. In example, we estimate the shift in angle of the birefringent strand to 13 degrees in our simulations, which should easily be detectable by optical methods.

In terms of experimental realization, we would suggest keeping the ratio of the outlet lengths below 2 and also to join them on the micro scale. Together with alertness towards unsteady flows, this should give optimal conditions for catastrophes occurring at reproducible conditions.

Finally we would like to compare between the micro-rheometer based on birefringence, and the proposed rheometer. Both concern extensional rheology, can be scaled down and are applicable for inline use, but as listed in table 4 there are also a number of significant differences.

Figure 5: (a) shows how the system is set in one of the states (#1 to #2), while the asymmetry is flipped in (b) (#3) such that a catastrophe occurs, when the bifurcation parameter is decrease (#4 to #5). The catastrophe is associated with a drop in hydraulic resistance as illustrated in (c).

Figure 6: The asymmetric cross-slot geometry is sketched with different inlet flow rates as well outlet lengths.

Figure 7: The flow rates \( Q_1 \) and \( Q_2 \) are varies slowly in time to produce the conditions described in section 4.
We \[ \phi / (Q_1 + Q_2) \]

\[ T_{\text{step}} = 1000 \]
\[ T_{\text{step}} = 2000 \]
\[ T_{\text{step}} = 4000 \]

Figure 8: The dissipation in the asymmetric cross-slot is shown as a function of Weissenberg number for a quasi-steady calculation with insets showing the trace of the conformation tensor on a logarithmic scale together with streamlines in red. The numbers in green correspond to those in figure 7 with the catastrophe between #4 and #5. We show results for three different speeds of these transient simulations (\( T_{\text{step}} \)) to verify, that the time scale of the jump is independent of this. The simulation is performed with 263k degrees of freedom.

<table>
<thead>
<tr>
<th>Property</th>
<th>Proposed</th>
<th>Birefringence [3]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dilute fluids</td>
<td>×</td>
<td>✓</td>
</tr>
<tr>
<td>Concentrated fluids</td>
<td>✓</td>
<td>×</td>
</tr>
<tr>
<td>Simple setup</td>
<td>✓</td>
<td>×</td>
</tr>
<tr>
<td>Gives a curve</td>
<td>×</td>
<td>✓</td>
</tr>
<tr>
<td>Bistability is a feature limitation</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 1: Two extensional micro-rheometers are compared, the proposed and the one based on birefringence [3].

6. Conclusion

We have described the background for generating catastrophes in bistable viscoelastic systems on a general level and presented simulation results in which the inlet flow rates in the cross-slot geometry is used as parameters to generate the catastrophe. Finally, we have discussed pros and cons for the suggested rheometer as well as provided guidelines for experimental verification.

References

[12] C. Multiphysics, User’s guide, version 3.5 a, COMSOL AB.