Elastic-driven instabilities in microfluidic flow-focusing devices

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Instabilities at the microscale: **Cross-Slot**

- **Experimental**
  - PRL 96, 144502 (2006)
  - Physical Review Letters
  - Elastic Instabilities of Polymer Solutions in Cross-Channel Flow
    - P.E. Arratia,1,2 C.C. Thomas,1 J. Diorio,1 and J.P. Gollub1,2

- **Numerical**
  - Physical Review Letters
  - Purely Elastic Flow Asymmetries
    - R.J. Poole,1 M.A. Alves1,2 and P.J. Oliveira3

**Newtonian:**
- Re < 10^-2

**PAA Boger fluid:**
- Re < 10^-2 (De=4.5)

**UCM model**
- 2D, Creeping Flow
Instabilities at the microscale: T-Channel


Investigating the stability of viscoelastic stagnation flows in T-shaped microchannels

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**Without** Cavity

**Pinned** stagnation point

\[ 0.075 \text{ wt. \% PEO in glycerol/water solution (60/40 wt. \%)} \]

**With** Cavity

**Free** stagnation point

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\( Q \rightarrow \frac{L}{w} \rightarrow 2Q \rightarrow \frac{L}{w} \rightarrow \frac{L}{w} \rightarrow Q \rightarrow Q \)
Flow focusing geometry

- **Operational Variables**
  
  \[ Q_1, Q_2 \]
  
  \[ Q_3 = 2 \times Q_2 + Q_1 \]

- **Dimensionless Variables**
  
  \[ FR = \frac{Q_2}{Q_1} \]
  
  \[ VR = \frac{U_2}{U_1} \quad (= FR) \]
  
  \[ Re = \frac{\rho U_2 D}{\eta_0} \]
  
  \[ De = \lambda \frac{U_2}{D} \]
  
  \[ El = \frac{De}{Re} \]

- **Channel dimensions:**
  
  - kept constant for all experiments and numerical calculations
  
  - Equal dimensions for all inlet/outlet arms
Fabrication process: **soft lithography**

1. **Silicon Wafer**
2. Spin coat photoresist **SU-8** and prebake
3. Spin coat **barrier coat** *(CEM-BC7.5)* and **contrast enhancer** *(CEM 388SS)* (vertical walls).
4. **Chrome Mask** over coated wafer
5. **UV Exposure** – *cross-link* **SU-8**
6. Wash **barrier coat** and **contrast enhancer**
7. Post-bake and develop **SU-8**
8. Pour **PDMS** over substrate and cure (80°C, 25 mins)
9. Peel off substrate
10. Seal with glass slide covered with PDMS

**Microchannels:**
- Planar geometry
- Square cross-section
- Nearly vertical walls
- Accuracy of channels to within 5%

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Experimental set-up

**Visualizations**
- **Microscope:** Leica, DMI LED
- **Camera:** Leica, DFC 350X
- **Objective lens:** 10× objective, NA=0.3 (δz=30µm)
- **Illumination:** Mercury lamp (λ=532nm)
- **Filter Cube:**
  - Emission filter: BP 530-545 nm
  - Dichroic mirror: 565 nm
  - Barrier filter: 610-675 nm
- **Tracers:** 1.1µm Nile red fluorescent particles (Ex/Em: 520/580 nm)
- **Additives:** SDS (0.1 wt.%)

**Flow**
- **Syringe pump:** CETONI, neMESYS with 3 independent modules
- **Flow rate:** 0.001 ≤ Q ≤ 3 ml/h
- **Syringes:** Hamilton Gastight syringes

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Hamilton gastight syringes

Three module Syringe pump

Inflow

Outflow

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Shear Rheology

- **Viscoelastic Fluid:**
  Aqueous solution of PAA ($M_w=18\times10^6$ g/mol)
  - **PAA 125 + NaCl**
    - 125 ppm PAA
    - 1% NaCl (wt)
    - 0.1% SDS (wt)

- **Newtonian Fluid:**
  - **Water**
    - Water
    - 0.1% SDS (wt)

**Steady Shear**
Anton Paar, model Physica MCR 301
Cone-and-plate geometry ($d=75\text{mm}$, $1^\circ$)

Based on 20× the minimum measurable torque ($1\times10^{-7}$ Nm)

Onset of inertial instabilities

$T = 20^\circ C$
Extensional Rheology

Haake CaBER 1, Thermo Electron Corporation
($D_p = 6$ mm)

**Aspect ratios:**
- $\Lambda_i = D_i/D_p = 0.33$
- $\Lambda_f = D_f/D_p = 1.56$

**Imposed strain:**
$$\varepsilon = \ln(\Lambda_f/\Lambda_i) = 1.53$$

**Fluid properties**

<table>
<thead>
<tr>
<th></th>
<th>PAA 125 + NaCl</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zero-shear rate viscosity</td>
<td>$\eta_0$ [Pa s]</td>
</tr>
<tr>
<td>CaBER relaxation time</td>
<td>$\lambda_{CaBER}$ [ms]</td>
</tr>
<tr>
<td>Density</td>
<td>$\rho$ [kg/m$^3$]</td>
</tr>
</tbody>
</table>

**T = 20ºC**

$$\frac{D}{D_0} \sim \exp\left(-\frac{t}{3\lambda}\right)$$

**Minimum resolvable diameter**
Governing equations

- Isothermal Incompressible Flow

\[ \nabla \cdot \mathbf{u} = 0 \]

Conservation of mass

\[ -\nabla p + \nabla \cdot \boldsymbol{\tau} + \eta_s \nabla^2 \mathbf{u} = 0 \]

Conservation of momentum

- Constitutive Equations

\[
\begin{bmatrix}
\lambda \epsilon \\
1 + \frac{\lambda \epsilon}{\eta_p} \text{tr}(\boldsymbol{\tau})
\end{bmatrix}
\nabla \cdot \boldsymbol{\tau} = 2\eta_p \mathbf{D}
\]

Simplified PTT model

\[ \epsilon = 0 \]

Oldroyd-B model

\[ \eta_s = 0 \]

UCM model

\[ \lambda = 0 \]

Newtonian fluid
Numerical method

- **Finite Volume Method**, using a time-marching algorithm*
  - Governing equations discretized in time over a small time step, \( \delta t \)
  - Differential equations integrated over control volumes, CV

- **Log-conformation approach** to solve the equivalent form of the constitutive equation containing an evolution equation of the conformation tensor.

* Oliveira et al., JNNFM, 79 (1998) 1-43
Afonso et al., JNNFM, submitted (2008)

- Implicit first-order Euler scheme for time-derivative discretization.

- Central differences for discretization of diffusive terms.

- **CUBISTA*** high-resolution scheme for discretization of the advective terms of the momentum equations.


- Pressure-velocity and velocity-stress coupling ensured at the CV faces – SIMPLEC algorithm****

**** Patankar and Spalding, Int. J. Heat and Mass Transfer, 15 (1972) 1787–806

- The ensemble of all control volumes defines the computational mesh.
Numerical mesh and boundary conditions

- **Mesh Characteristics:**
  - Two-dimensional
  - Structured, orthogonal and non-uniform
  - Dimensions equal to the experiments

- **Boundary Conditions:**
  - **INLET**
    - Fully-developed velocity profile
    - Null stress components
  - **OUTLET**
    - Vanishing streamwise gradients of velocity and stress components
    - Constant pressure gradient
  - **WALLS**
    - No-slip conditions

**Standard Mesh used**
(more refined meshes also used)

<table>
<thead>
<tr>
<th>Geometry</th>
<th>NCells</th>
<th>$\Delta x_{\text{min}}$, $\Delta y_{\text{min}}$, $\Delta z_{\text{min}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D</td>
<td>23001</td>
<td>0.02$D$</td>
</tr>
</tbody>
</table>
Converging Flow

- Two opposing lateral streams shape a third inlet stream
- Converging flow region
- Separation streamlines naturally evolve to a nearly hyperbolic shape
- Hencky strain controlled by operating parameters:

\[ \varepsilon = \ln \left( \frac{D_1}{D_3} \right) = \ln \left( \frac{3}{2} (1 + 2 \cdot VR) \right) \]

- Approximately constant strain rate at the centerline
Two opposing lateral streams shape a third inlet stream

Converging flow region

Separation streamlines naturally evolve to a nearly hyperbolic shape

Hencky strain controlled by operating parameters:

$$\varepsilon_H = \ln\left(\frac{D_1}{D_3}\right) = \ln\left[\frac{3}{2} (1 + 2 \cdot VR)\right]$$

Approximately constant strain rate at the centerline
Instabilities at the microscale

Purely elastic flow asymmetries in flow-focusing devices

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UCM model
2D, Creeping Flow

For \textbf{low} VR: asymmetric flow not observed

For \textbf{high} VR: \textit{symmetric} $\rightarrow$ \textit{asymmetric} $\rightarrow$ \textit{oscillatory}

- The critical $De_c$ becomes approximately \textbf{constant}: $De_c \sim 0.33$
- \textbf{Bistable} flow
Effect of VR on the degree of asymmetry

\[ F^* = \frac{F_W - F_E}{F_3} \]

- \( F^* = 0 \) (symmetric flow)
- \( F^* \) progressively deviates from \( F^* = 0 \) as the flow becomes increasingly asymmetric.

For high VR:
- \( De_c \) independent of VR
- Evolution of asymmetry independent of VR
- Supercritical pitchfork bifurcation:
  \[ F^* = a\sqrt{De - De_c} \]
  \[ = 0.59\sqrt{De - 0.33} \]

Oliveira et al., JNNFM, 160 (2009) 31-39
Effect of $\beta$ on the degree of asymmetry

$$\beta \equiv \frac{\eta_s}{\eta_0} = \frac{\eta_s}{\eta_s + \eta_p}$$

$$F^* = \frac{F_W - F_E}{F_3}$$

$F^* = 0$ (symmetric flow)

$F^*$ progressively deviates from $F^* = 0$ as the flow becomes increasingly asymmetric.

- $\beta$ has a stabilizing effect on the flow:
  - Increase in the critical $De_c$
  - For $\beta \geq 6/9$, no steady asymmetry is observed.
Effect of $\varepsilon$ on the degree of asymmetry

$$F^* = \frac{F_W - F_E}{F_3}$$

$F^*$ = 0 (symmetric flow)

$F^*$ progressively deviates from $F^* = 0$ as the flow becomes increasingly asymmetric.

- Increase in the critical $De_c$
- Decrease in the degree of asymmetry ($\varepsilon < 0.04$)
- For $\varepsilon \geq 0.04$, the steady asymmetry no longer observed. The flow transitions directly from steady symmetric to unsteady.
Axial Normal Stress Profiles

- Similar levels of normal stresses achieved near critical conditions.

- Extensional properties decisive for the onset of flow asymmetry.
Viscoelastic Fluid: PAA125+NaCl

\[ Q_1 = 0.01 \text{ ml/h} \]

increasing \( Q_2 \)

\( Q_2 = 0.05 \text{ ml/h, } VR = 5 \)
\[ Re = 0.23, \; De = 0.38 \]

\( Q_2 = 0.2 \text{ ml/h, } VR = 20 \)
\[ Re = 0.87, \; De = 1.41 \]

\( Q_2 = 0.5 \text{ ml/h, } VR = 50 \)
\[ Re = 2.15, \; De = 3.479 \]

Symmetric

Steady Asymmetric

Unsteady 3D
Viscoelastic Fluid: PAA125+NaCl

\[ Q_1 = 0.01 \text{ ml/h} \]

- \[ Q_2 = 0.05 \text{ ml/h}, \ VR = 5 \]
  - \( Re = 0.23, \ De = 0.38 \)

- \[ Q_2 = 0.1 \text{ ml/h}, \ VR = 10 \]
  - \( Re = 0.45, \ De = 0.723 \)

- \[ Q_2 = 0.2 \text{ ml/h}, \ VR = 20 \]
  - \( Re = 0.87, \ De = 1.41 \)
Viscoelastic Fluid: **PAA125+NaCl**

- For $Q_1 = 0.01$ ml/h:
  - **Experimental**: [Image 1]

- For $Q_2 = 0.05$ ml/h, $VR = 5$:
  - **Re** = 0.23, **De** = 0.38
  - **UCM**: [Image 2]

- For $Q_2 = 0.1$ ml/h, $VR = 10$:
  - **Re** = 0.45, **De** = 0.723
  - **UCM**: [Image 3]

- For $Q_2 = 0.2$ ml/h, $VR = 20$:
  - **Re** = 0.87, **De** = 1.41
  - **UCM**: [Image 4]
Viscoelastic Model

$Q_1 = 0.01 \text{ ml/h}$

UCM 2D Calculations

$Q_2 = 0.05 \text{ ml/h, } VR = 5$
$Re = 0.23, \ De = 0.38$

Oldroyd-B 2D Calculations

$Q_2 = 0.2 \text{ ml/h, } VR = 20$
$Re = 0.87, \ De = 1.41$

$Q_2 = 0.35 \text{ ml/h, } VR = 35$
$Re = 0.87, \ De = 1.41$

Unsteady 3D
Experimental Flow Map

- **Experimental**
  - PAA 125 + NaCl

- **Numeric**
  - UCM Model
  - 2D, Creeping Flow
Summary

- Elastically-driven asymmetries at the microscale.

- **Symmetric-breaking bifurcation** at high $De$ and $VR$.

- **Unsteady 3D** flow above a critical $De$: useful for mixing purposes.

- Numerical 2D calculations reproduce qualitatively the experimental results.

**Ongoing work:**
- Experimental: μPIV
- Numerical: 3D simulations
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