PROGRAMME
PROGRAMME

Monday 5 April - Afternoon

12:30 Lunch

Session 1 Chairman: K Walters

14:00 - 14:40 D V Boger
Something old, something new, and something very new in industrial rheology

14:40 - 15:20 J R A Pearson
The role of diffusion in non-Newtonian fluid mechanics

15:20 - 15:45 D R Oliver
Simultaneous shear and squeezing flow applied to a ceramic paste

15:45 - 16:15 Coffee/Tea

Session 2 Chairman: K Walters

16:15 – 16:45 I Emri
The effect of boundary conditions on structure formation of PA fibers

16:45 - 17:15 G N Greaves
Solid state rheology of zeolites under thermobaric stress

17:15 - 17:40 B Debbaut
The double convected pom-pom model: a numerical validation for the contraction flow

17:40 - 18:05 E I Frenkin
Thermophysical characteristics of PP/LCP blends under high pressure

19:30 Dinner

27. Mar. 2004
Tuesday 6 April - Morning

Session 3  Chairman: M H Wagner

09:00 - 10:00  H M Laun  
Thirty years of industrial polymer rheology at BASF

10:00 - 10:25  P Moldenaers  
Morphology development of two-phase blends during capillary flow

10:25 - 10:55  Coffee/Tea

Session 4  Chairman: M H Wagner

10:55 - 11:35  C Gallegos  
Rheology of recycled-EVA modified bitumen

11:35 - 12:05  M P Escudier  
Experiments and numerical simulations of laminar viscoelastic flow through sudden expansions

12:05 – 12:30  J M Maia  
Influence of the operating conditions on the gelatinisation of rice flour during extrusion

12:30 - 14:00  Lunch
PROGRAMME

Tuesday 6 April - Afternoon

12:30 – 13:45 Lunch

Session 5  Chairman: A R Davies

13:45 - 14:40 H A Barnes
Thirty years of industrial dispersion rheology at Unilever

14:40 - 15:20 J-M Piau
Macro and micro rheometry of carbopol gels

15:20 - 15:45 H P Hürlimann
A new multipass-type polymer compounding machine approaches industrial application

15:45 - 16:15 Coffee/Tea

Session 6  Chairman: A R Davies

16:15 - 16:55 D G Baird
Rheology of highly filled polymers using squeezing flow

16:55 - 17:35 M H Wagner
Melt rheology of industrial polymers: relating stress to strain and energy

17:35– 18:00 O Kulikov
The use of thermoplastic and raw elastomers to delay the melt fracture onset in extrusion of polyethylene

19:00 for 19:30 Conference Dinner
Wednesday 7 April - Morning

Session 7    Chairman: P Townsend

09:00 - 09:40  G C Maitland
Complex fluids for hydrocarbon recovery - rheology *in extremus*

09:40 - 10:20  R Keunings
The CRAFT tube model: a new constitutive equation for blends of entangled linear polymers

10:20 - 10:45  Ch Bailly
Prediction of linear viscoelastic properties from molecular structure for blends of linear and x entangled polymers

10:45 - 11:15  Coffee/Tea

Session 8    Chairman: P Townsend

11:15 - 11:40  F T Pinho
Optimisation of profile extrusion dies: numerical and experimental work

11:40 - 12:00  F Chinestra
$\alpha$-NEM and model reduction: two new and powerful numerical techniques for simulating complex flows

12:00 - 12:30  O Wallevik
Rheology of coarse particle suspensions such as fresh concrete

12:30  End of Conference
Optimisation of Profile Extrusion Dies: Numerical and Experimental Work

O. S. Carneiro, J. M. Nóbrega
Departamento de Engenharia de Polímeros, Universidade do Minho

F. T. Pinho
C.E.F.T., Departamento de Engenharia Mecânica, Universidade do Minho

P. J. Oliveira
Departamento de Engenharia Electromecânica, Universidade da Beira Interior

Industrial Rheology
April 5th-7th, 2004
Chester, UK
Introduction

Motivation

Need to have a swifter, less dependent on personal knowledge design process

Objective

Development of an integrated ‘automatic’ extrusion die design code
Introduction

Development steps

• Define initial geometry

• Geometry and mesh generators

• Computational code base on the finite volume method (3D, viscoelastic (here purely viscous), thermal energy)

• Search method - Optimisation routine

• Evaluation of performance - Objective Function

Other requirements

• Maximum flow rate - shark skin

• Maximum angle of convergence - melt fracture (ext flows)

• Anticipation of post-extrusion effects

• Flow balancing - internal stresses

• Total pressure drop and hot spots
Flow balancing – Optimisation methodology

Pre-Processor

Geometry
Mesh

3D non-isothermal flow field calculation (FVM)

Velocity
Pressure
Temperature

Performance Evaluation

Modification of the controllable geometrical parameters until the optimum is reached

Industrial Rheology
April 5th–7th, 2004
Chester, UK
Flow balancing – Optimisation methodology

Trial Parameters

Pre-Processor

3D non-isothermal flow field calculation (FVM)

Performance Evaluation

Progressive mesh Refinements

Modification of the controllable geometrical parameters until the optimum is reached

Pent. IV / 2.4 GHz

<table>
<thead>
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<th>Number of Cells</th>
<th>Time [h:m:s]</th>
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<tr>
<td>6</td>
<td>272 220</td>
<td>1:12:17</td>
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<tr>
<td>8</td>
<td>593 928</td>
<td>4:28:36</td>
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<td>10</td>
<td>688 024</td>
<td>6:43:42</td>
</tr>
</tbody>
</table>

Industrial Rheology
April 5th-7th, 2004
Chester, UK
Flow balancing – Optimisation methodology

**Equations to Solve:**

**Cons. of mass:**
\[
\frac{\partial \rho u_j}{\partial x_j} = 0
\]

**Cons. of linear Momentum:**
\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}
\]

**Cons. of Energy:**
\[
\frac{\partial \rho c T}{\partial t} + \frac{\partial \rho c u_i T}{\partial x_i} = \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) + \tau_{ij} \frac{\partial u_i}{\partial x_j}
\]

**Constitutive equation:**
\[
\tau_{ij} = 2\eta\dot{\gamma}T S_{ij}
\]
Flow balancing – Optimisation methodology

\[ F_{obj} = \sum_{i=1}^{n} \left\{ \alpha \left( 1 - \frac{V_i}{V_{obj.i}} \right)^2 + k(1 - \alpha) \left[ 1 - \frac{(L/t)_i}{(L/t)_{min}} \right]^2 \right\} \frac{A_i}{A} \]

**Flow Balance**

\[ V_{obj.i} = \bar{V} \frac{A_{obj.i}}{A_i} \]

\( (L/t)_{min} \) - essential to reduce sensitivity of die

\( k = 0 \) when \((L/t)_i \geq (L/t)_{min} = 7\)

\( \alpha = 0.75 \)

**Advisable L/t value**

**Performance Evaluation**

**Pre-Processor**

**3D non-isothermal flow field calculation (FVM)**

**Trial Parameters**

**Area Weighting**

**Modification of the controllable geometrical parameters until the optimum is reached**

**Objective flow rate**

**ES required area in die**

**Velocity**

**Pressure**

**Temperature**

**Geometry**

**Mesh**
Flow balancing – Optimisation methodology

Trial Parameters

Pre-Processor

Geometry
Mesh

3D non-isothermal flow field calculation (FVM)

Velocity
Pressure
Temperature

Performance Evaluation

Modification of the controllable geometrical parameters until the optimum is reached

SIMPLEX Method (SM)

Experimental Method (EM)
Flow balancing – Optimisation methodology

Trial Parameters

Geometry

Pre-Processor

Mesh

3D non-isothermal flow field calculation (FVM)

Velocity

Pressure

Temperature

Performance Evaluation

\[ F_{obj} = \sum_{i=1}^{n} \left\{ \alpha \left( 1 - \frac{V_i}{V_{obj,i}} \right)^2 + k \left[ 1 - \alpha \left( \frac{L_i}{L_{min}} \right) \right]^2 \frac{A_i}{A} \right\} \]

Modification of the controllable geometrical parameters until the optimum is reached
Flow balancing – Optimisation strategies

- **Required Profile**: ST1 (length) and ST2 (thickness)

- **Optimisation Strategy**: Flow balancing – Optimisation strategies

- **Die Flow Channel**

- **Haul-off Speed**: 
  
- **Final Profile**

Mathematical expressions:

\[
\frac{V_3}{V_1} = \frac{V_3}{V_2}
\]

\[
\frac{V_3}{V_1} \neq \frac{V_3}{V_2}
\]
Case study - Geometry

Initial flow channel dimensions

<table>
<thead>
<tr>
<th>ES</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_i$ [mm]</td>
<td>2.0</td>
<td>2.5</td>
<td>2.5</td>
<td>3.0</td>
<td>2.0</td>
<td>4.0</td>
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<tr>
<td>$L_i$ [mm]</td>
<td>30.0</td>
<td>37.5</td>
<td>37.5</td>
<td>45.0</td>
<td>30.0</td>
<td>60.0</td>
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<tr>
<td>$L_i/t_i$</td>
<td>15.0</td>
<td>15.0</td>
<td>15.0</td>
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<td>15.0</td>
<td>15.0</td>
</tr>
</tbody>
</table>
Case study – Modelling data

Viscosity function (PP)

\[
\eta(\dot{\gamma}, T) = F(\dot{\gamma} \times H(T)) H(T)
\]

\[
F(\dot{\gamma}) = \eta_\infty + \frac{\eta_0 - \eta_\infty}{\left(1 + (\lambda \dot{\gamma})^2\right)^{1/2}} \quad H(T) = \exp\left[\beta\left(\frac{1}{T} - \frac{1}{T_{\alpha}}\right)\right]
\]

Operating and thermal boundary conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>Flow rate*</td>
<td>20 kg/h</td>
</tr>
<tr>
<td>Melt inlet temperature</td>
<td>230 °C</td>
</tr>
<tr>
<td>Outer die walls temperature</td>
<td>230 °C</td>
</tr>
<tr>
<td>Inner (mandrel) die walls</td>
<td>Adiabatic</td>
</tr>
</tbody>
</table>

* Corresponding to an average velocity of 1 m/min at the die exit

Optimisations performed

**DieL** – Length optimisation

**DieT** – Thickness optimisation
Case study – Optimisation

DieL

Cells Along Thickness

Calculation Time [hh:mm] ▼ - Mesh Refinement

DieT

Cells Along Thickness

Calculation Time [hh:mm] ▼ - Mesh Refinement

Industrial Rheology
April 5th-7th, 2004
Chester, UK
Case study – Optimisation

DieL

Cells Along Thickness

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<td>10%</td>
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<td>20%</td>
<td>25%</td>
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<td>0:01</td>
<td>0:01</td>
<td>0:02</td>
<td>0:02</td>
<td>0:03</td>
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<td>0:25</td>
<td>0:38</td>
<td>0:52</td>
<td>1:20</td>
<td>2:02</td>
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Calculation Time [hh:mm]

Difference to Final Solution

Mesh Refinement

DieL

Cells Along Thickness

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<td>0:02</td>
<td>0:02</td>
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<td>0:25</td>
<td>0:38</td>
<td>0:52</td>
<td>1:20</td>
<td>2:02</td>
</tr>
</tbody>
</table>

Calculation Time [hh:mm]

Difference to Final Solution

Mesh Refinement
Case study – Dies tested
Case study – Flow distribution

Velocity [m/s]

DieIni  DieL  DieT

Industrial Rheology
April 5th-7th, 2004
Chester, UK
# Case study – Experimental validation

## Extrusion experiments performed

<table>
<thead>
<tr>
<th>Run ID</th>
<th>Extrusion Die</th>
<th>Mass Flow Rate [kg/h]</th>
<th>Die Wall Temperature [° C]</th>
<th>Average Melt Exit Velocity [m/min]</th>
</tr>
</thead>
<tbody>
<tr>
<td>INI</td>
<td>DieINI</td>
<td>20.4</td>
<td>230</td>
<td>0.99</td>
</tr>
<tr>
<td>L1</td>
<td>DieL</td>
<td>19.8</td>
<td>230</td>
<td>0.96</td>
</tr>
<tr>
<td>L2</td>
<td>DieL</td>
<td>19.7</td>
<td>250</td>
<td>0.95</td>
</tr>
<tr>
<td>L3</td>
<td>DieL</td>
<td>13.8</td>
<td>230</td>
<td>0.67</td>
</tr>
<tr>
<td>T</td>
<td>DieT</td>
<td>19.3</td>
<td>230</td>
<td>0.90</td>
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</table>

## Pressure Drop - Numerical predictions and measured values

<table>
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<tr>
<th>Run ID</th>
<th>Pressure Drop</th>
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<tbody>
<tr>
<td></td>
<td>Predicted [MPa]</td>
</tr>
<tr>
<td>INI</td>
<td>3.65</td>
</tr>
<tr>
<td>L1</td>
<td>2.56</td>
</tr>
<tr>
<td>L2</td>
<td>2.48</td>
</tr>
<tr>
<td>L3</td>
<td>2.31</td>
</tr>
<tr>
<td>T</td>
<td>3.65</td>
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</tbody>
</table>
## Case study – Experimental validation

### Relative elemental cross-section areas

<table>
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<tr>
<th>Run ID</th>
<th>ES1</th>
<th>ES2+3</th>
<th>ES4</th>
<th>ES5</th>
<th>ES6</th>
</tr>
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<tr>
<td>INI</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M</td>
<td>3.2</td>
<td>18.3</td>
<td>19.2</td>
<td>7.1</td>
<td>52.2</td>
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<tr>
<td>P</td>
<td>2.9</td>
<td>16.2</td>
<td>19.2</td>
<td>6.7</td>
<td>55.0</td>
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<tr>
<td>D</td>
<td>-9.4%</td>
<td>-11.5%</td>
<td>0.0%</td>
<td>-5.6%</td>
<td>5.4%</td>
</tr>
<tr>
<td>U</td>
<td>9.0%</td>
<td>9.5%</td>
<td>4.2%</td>
<td>14.2%</td>
<td>3.9%</td>
</tr>
<tr>
<td>L1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M</td>
<td>8.3</td>
<td>26.0</td>
<td>18.7</td>
<td>18.2</td>
<td>28.7</td>
</tr>
<tr>
<td>P</td>
<td>8.2</td>
<td>25.4</td>
<td>19.1</td>
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<td>-1.0%</td>
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<tr>
<td>U</td>
<td>6.7%</td>
<td>4.9%</td>
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<td>8.8%</td>
<td>3.9%</td>
</tr>
<tr>
<td>T</td>
<td></td>
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<tr>
<td>M</td>
<td>7.4</td>
<td>26.2</td>
<td>20.2</td>
<td>20.2</td>
<td>26.0</td>
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<tr>
<td>P</td>
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<tr>
<td>D</td>
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<td>-1.5%</td>
<td>-2.5%</td>
<td>0.5%</td>
<td>3.1%</td>
</tr>
<tr>
<td>U</td>
<td>6.3%</td>
<td>4.4%</td>
<td>4.9%</td>
<td>8.2%</td>
<td>5.6%</td>
</tr>
</tbody>
</table>

Measured (M), Predicted (P), Difference (D), Uncertainty (U)
Case study – Length vs thickness optimisation

Flow channel dimensions

<table>
<thead>
<tr>
<th></th>
<th>ES1</th>
<th>ES2</th>
<th>ES3</th>
<th>ES4</th>
<th>ES5</th>
<th>ES6</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_i$ [mm]</td>
<td>2.0</td>
<td>2.5</td>
<td>2.5</td>
<td>3.0</td>
<td>2.0</td>
<td>4.0</td>
</tr>
<tr>
<td>$L_i$ [mm]</td>
<td>30.0</td>
<td>37.5</td>
<td>37.5</td>
<td>45.0</td>
<td>30.0</td>
<td>60.0</td>
</tr>
<tr>
<td>$L_i/t_i$</td>
<td>15.0</td>
<td>15.0</td>
<td>15.0</td>
<td>15.0</td>
<td>15.0</td>
<td>15.0</td>
</tr>
<tr>
<td>$t_i$ [mm]</td>
<td>2.0</td>
<td>2.5</td>
<td>2.5</td>
<td>3.0</td>
<td>2.0</td>
<td>4.0</td>
</tr>
<tr>
<td>$L_i$ [mm]</td>
<td>7.50</td>
<td>11.50</td>
<td>11.50</td>
<td>17.50</td>
<td>7.00</td>
<td>60.00</td>
</tr>
<tr>
<td>$L_i/t_i$</td>
<td>3.75</td>
<td>4.60</td>
<td>4.60</td>
<td>3.83</td>
<td>3.5</td>
<td>15.0</td>
</tr>
<tr>
<td>$t_i$ [mm]</td>
<td>2.42</td>
<td>2.64</td>
<td>2.64</td>
<td>2.89</td>
<td>2.42</td>
<td>3.19</td>
</tr>
<tr>
<td>$L_i$ [mm]</td>
<td>30.0</td>
<td>37.5</td>
<td>37.5</td>
<td>45.0</td>
<td>30.0</td>
<td>60.0</td>
</tr>
<tr>
<td>$L_i/t_i$</td>
<td>12.40</td>
<td>14.20</td>
<td>14.20</td>
<td>15.57</td>
<td>12.40</td>
<td>18.81</td>
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</tbody>
</table>

DieIni  DieL  DieT
Case study – Length vs thickness optimisation

<table>
<thead>
<tr>
<th>Extrusion Die</th>
<th>ES1</th>
<th>ES2</th>
<th>ES3</th>
<th>ES4</th>
<th>ES5</th>
<th>ES6</th>
</tr>
</thead>
<tbody>
<tr>
<td>DieINI</td>
<td>6.20</td>
<td>3.72</td>
<td>3.39</td>
<td>2.18</td>
<td>7.46</td>
<td>1.00</td>
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<tr>
<td>DieL</td>
<td>1.08</td>
<td>1.15</td>
<td>1.03</td>
<td>1.12</td>
<td>1.15</td>
<td>1.00</td>
</tr>
<tr>
<td>DieT</td>
<td>1.68</td>
<td>1.38</td>
<td>1.33</td>
<td>1.24</td>
<td>1.56</td>
<td>1.00</td>
</tr>
</tbody>
</table>

After stress relax in oven
Conclusion

• Optimisation algorithm improved significantly the extrusion die flow distribution;

• Code predicted accurately melt flow distribution and the pressure drop;

• Length control leads to higher sensitivity to processing conditions than thickness control;

• Thickness control extrudates have higher propensity to distort.

Next steps

• Calibrator and cooling units (done)

• Free surface routines (to be done)

• Viscoelastic (under way)
Case study – Flow distribution optimisation

<table>
<thead>
<tr>
<th></th>
<th>DieL</th>
<th>DieT</th>
</tr>
</thead>
<tbody>
<tr>
<td>ES1</td>
<td>0.98</td>
<td>1.02</td>
</tr>
<tr>
<td>ES2</td>
<td>0.93</td>
<td>0.97</td>
</tr>
<tr>
<td>ES3</td>
<td>1.04</td>
<td>0.99</td>
</tr>
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<td>ES4</td>
<td>0.95</td>
<td>0.99</td>
</tr>
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<td>ES5</td>
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<td>ES6</td>
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